Conformations of N-Heterocyclic Carbene Ligands in Ruthenium Complexes Relevant to Olefin Metathesis

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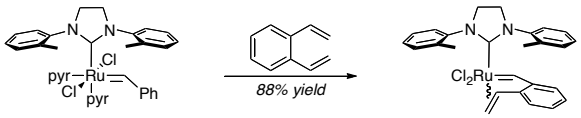
Supporting Information

Experimental Section: Synthesis

General. All glassware was either oven dried or flame dried, and reactions were done under an atmosphere of argon or in a nitrogen-filled glovebox unless otherwise noted. All organic solvents were dried by passage through solvent purification columns containing activated alumina. All commercial chemicals were used as obtained. Divinylbezene was prepared according to literature procedure.[2] High-resolution mass spectrometry (HRMS) data were obtained on a JEOL MSRoute mass spectrometer.



4 **5**

Preparation of π-Complex 5. In a nitrogen-filled glovebox, a 20 mL scintillation vial was charged with **4** (0.16 g, 0.24 mmol) and benzene (4 mL). A solution of 1,2-divinylbenzene (0.034 mg, 0.26 mmol) in benzene (4 mL) was then added. The vial was capped and stored in the glovebox at r.t. for 18 h. The resulting burnt orange solution was decanted, leaving a green crystalline solid. The solid was removed from the glovebox, washed with pentane (2 x 2 mL), and dried under vacuum, yielding 0.11 g (88%). See pages S12-S29 for NMR characterization data. HR-MS (FAB+) Calculated for $C_{26}H_{26}N_2Cl_2Ru$, 538.0517; found, 538.0518.

Experimental Section: NMR Spectroscopy Experiments

NMR spectra were obtained on a Bruker Avance DPX 400 MHz NMR spectrometer equipped with a 5 mm dual $^1H/^{13}C$ Z-gradient probe. Unless otherwise specified, spectra were obtained at 23 °C. For experiments requiring low temperatures, the probe was calibrated with a sample of methanol containing a trace amount of gaseous HCl.[3] 1D ^1H and ^{13}C spectra were acquired with standard pulse sequences and parameters. Details for the 2D experiments are as follows:

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[2] Mitchell, R. H.; Ghose, B. N.; Williams, M. E. *Can. J. Chem.* **1977**, *55*, 210.
[3] Braun, S.; Kalinowski, H. –O.; Berger, S. *150 and More NMR Experiments: A Practical Course*; Wiley-VCH: Weinheim, 1998.

Gradient-enhanced 2D COSY experiment.[4] The **cosygs** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 7.01 Hz/pt. 256 FIDs recorded, each consisting of 4 scans and 1024 data points (AQ = 0.071 s). A recycle delay of (D1) of 1.5 s was employed. Processing parameters: unshifted sinusoidal apodization was applied in both dimensions prior to the Fourier transformation.

2D COSYLR experiment.[5] The **cosylr** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 7.01 Hz/pt. 128 FIDs recorded, each consisting of 8 scans and 1024 data points (AQ = 0.071 s). Refocusing delays of 100 ms and 200 ms were used in separate experiments. A recycle delay of (D1) of 2.0 s was employed. Zero-filling was applied once to achieve digital resolution of 3.5 Hz/pt in each dimension. Processing parameters: unshifted sinusoidal (SINE, SSB=0) apodization was applied in both dimensions prior to the Fourier transformation.

2D ROESY experiment.[6] The **roesytp.2** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 7184 Hz. F2 and F1 digital resolution, 3.5 Hz/pt. 256 FIDs recorded, each consisting of 16 scans and 2048 data points (AQ = 0.142 s). The 800 ms spin lock consisted of 5404 cycles of phase-shifted pairs of 74 μs 180° pulses. A recycle delay of (D1) of 2.0 s was employed. Processing parameters: $\pi/2$ shifted sine^2 (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

Representative 2D NOESY/EXSY experiment.[7] The **noesytp** pulse program was used with the following acquisition parameters. F2 and F1 sweep widths, 2913 Hz. F2 and F1 digital resolution, 2.8 Hz/pt. 256 FIDs recorded, each consisting of 8 scans and 1024 data points (AQ = 0.176 s). A mixing time of 800 ms was set as a simple delay. A recycle delay of (D1) of 2.0 s was employed. Processing parameters: $\pi/2$ shifted sine^2 (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

Gradient-enhanced 2D ^{1}H-^{13}C HMQC experiment.[8] The **inv4gp** pulse program was used with the following acquisition parameters. F2 sweep width, 7184 Hz, F1 sweep width, 32,895 Hz. F2 digital resolution, 7.01 Hz/pt, F1 digital resolution, 257 Hz/pt. 128 FIDs recorded, each consisting of 16 scans and 1024 data points (AQ = 0.071 s). The D2 delay was set to 3.57 ms (1/2J = 140 Hz). A recycle delay (D1) of 3.0 s was employed. Processing parameters: Zero-filling was applied once (SI = 2048) in F2 to achieve a digital resolution of 3.5 Hz/pt and eight times (SI = 1024) in F1 to achieve a digital resolution of 32 Hz/pt. Exponential (EM, LB = 5) apodization was applied in the F2 dimension and $\pi/3$ shifted sine^2 (QSINE, SSB=3) apodization was applied in the F1 dimension prior to the Fourier transformation.

2D ^{1}H-^{13}C HMQC experiment without F2 decoupling.[9] The **inv4nd** pulse program was used with the following acquisition parameters. F2 sweep width, 4789 Hz, F1 sweep width, 17605 Hz. F2 digital resolution, 4.68 Hz/pt, F1 digital resolution, 137.5 Hz/pt. 128 FIDs recorded, each consisting of 64 scans and 1024 data points (AQ = 0.107 s). The D2 delay was set to 3.57 ms (1/2J = 140 Hz). A recycle delay (D1) of 2.2 s was employed. Processing parameters: Zero-filling was applied eight times (SI = 1024) in F1 to achieve a digital resolution of 17.2 Hz/pt. Processing parameters: $\pi/2$ shifted sine^2 (QSINE, SSB=2) apodization was applied in both dimensions prior to the Fourier transformation.

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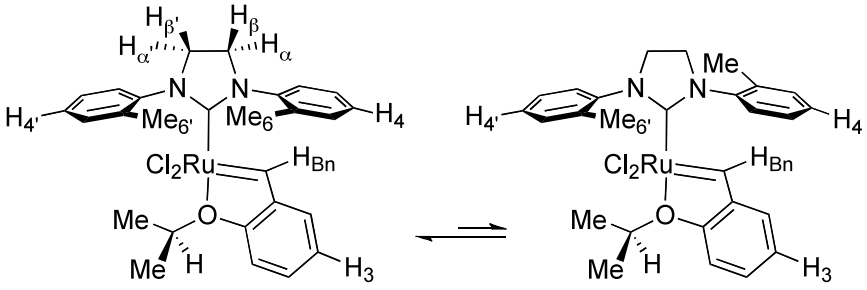
[4] Hurd, R. *J. Magn. Reson.* **1990**, *87*, 422.
[5] Bax, A.; Freeman, R. *J. Magn. Reson.* **1981**, *44*, 542.
[6] Hwang, T. –L.; Shaka, A. J. *J. Am. Chem. Soc.* **1992**, *114*, 3157.
[7] Jeener, J.; Meier, B. H.; Bachmann, P.; Ernst, R. R. *J. Chem. Phys.* **1979**, *71*, 4546.
[8] Hurd, R. E.; John, B. K. *J. Magn. Reson.* **1991**, *91*, 648.
[9] Bax, A.; Griffey, R. H.; Hawkins, B. L. *J. Magn. Reson.* **1983**, *55*, 301.

NMR Analysis of Benzylidene 3



3a **3b**

400 MHz ^{1}H NMR (CD_2Cl_2, 19 °C): 16.45 ppm (1H, s), 8.57 (1H, br s), 7.58-7.18 (8H, m), 6.89 (3H, app d), 4.95 (1H, sept, J = 6.1 Hz), 4.37 (2H, br s), 4.08 (2H, br s), 2.51 (6H, s), 1.47-1.22 (6H, br m).

400 MHz ^{1}H NMR for major isomer **3a** (CD_2Cl_2, –48 °C): 16.37 ppm (1H, s, H_{Bn}), 8.54 (1H, d, J = 7.4 Hz, $H_{2'}$), 7.6-7.3 (8H, m), 7.20 (1H, t, J = 7.5 Hz), 6.9-6.8 (3H, m), 4.94 (1H, sept, J = 6.1 Hz), 4.40 (2H, m), 4.10-3.95 (2H, m), 2.51 (3H, s), 2.45 (3H, s), 1.38 (3H, d, J = 5.9 Hz), 1.23 (3H, d, J = 5.9 Hz). Minor isomer **3b**: 16.40 (1H, s).

100 MHz ^{13}C NMR for major isomer **3a** (CD_2Cl_2, –48 °C):

peak #	freq. (Hz)	freq. (ppm)	intensity	intensity(absolute)
1	29752.299	295.7111	0.048685	332095.316000
2	21038.855	209.1073	0.054215	369815.912000
3	15355.857	152.6234	0.068693	468574.648000
4	14466.597	143.7849	0.083085	566745.924000
5	14256.821	141.7000	0.072214	492592.968000
6	14223.297	141.3668	0.080313	547837.092000
7	13889.728	138.0514	0.068631	468150.220000
8	13858.516	137.7412	0.084934	579357.184000
9	13270.839	131.9002	0.110824	755962.288000
10	13226.277	131.4573	0.115626	788718.888000
11	13117.935	130.3805	0.132291	902394.936000
12	13094.956	130.1521	0.109696	748267.324000
13	13021.910	129.4261	0.105835	721928.328000
14	12975.180	128.9616	0.100812	687669.788000
15	12961.729	128.8279	0.100074	682631.548000
16	12911.829	128.3320	0.113653	775261.520000
17	12863.458	127.8512	0.117171	799259.664000
18	12363.549	122.8825	0.120276	820438.720000
19	12297.960	122.2306	0.105240	717874.680000
20	11424.603	113.5503	0.109218	745004.580000
21	7562.637	75.1658	0.113104	771513.176000
22	5529.377	54.9570	0.302563	2063864.884000
23	5502.151	54.6864	0.695672	4745374.464000
24	5474.793	54.4145	0.929770	6342223.296000
25	5447.567	54.1439	0.720516	4914840.220000
26	5420.213	53.8720	0.314864	2147778.584000
27	5218.730	51.8695	0.097512	665156.928000
28	2221.267	22.0774	0.122898	838325.308000
29	2196.144	21.8277	0.127974	872945.216000
30	1962.093	19.5014	0.120911	824767.136000
31	1840.543	18.2933	0.111360	759618.572000

100 MHz ^{13}C NMR for minor isomer **3b** (CD_2Cl_2, –48 °C): 297.31 ppm.

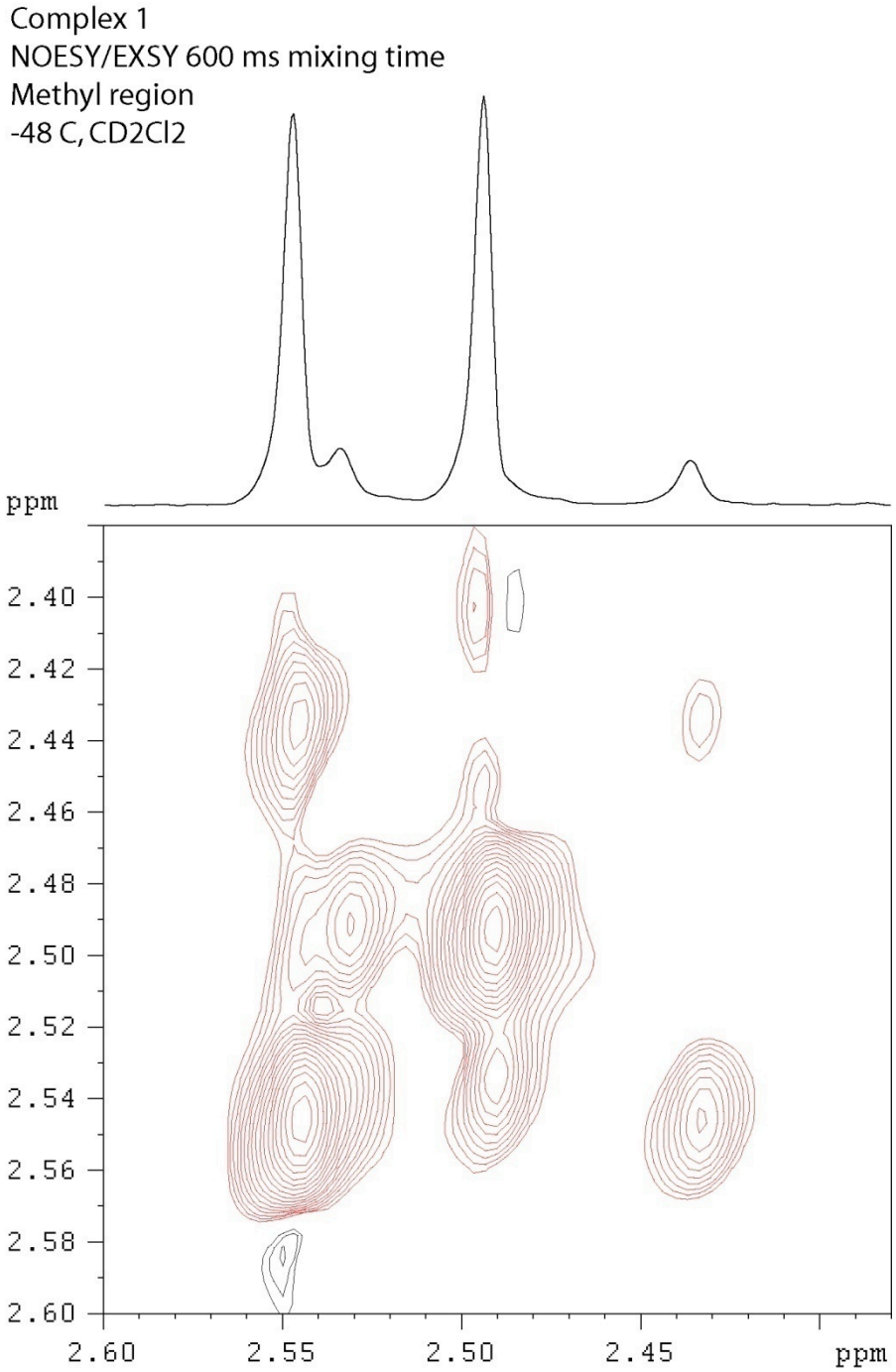


Figure S1. 400 MHz ^{1}H NOESY/EXSY spectrum of the methyl region for complex **3** dissolved in CD2Cl2 at -48 °C. Exchange between major and minor forms is evident; this data set was used to extract the magnetization exchange rate constant (k_{for}) between major and minor forms to be 3.9 s^{-1}.

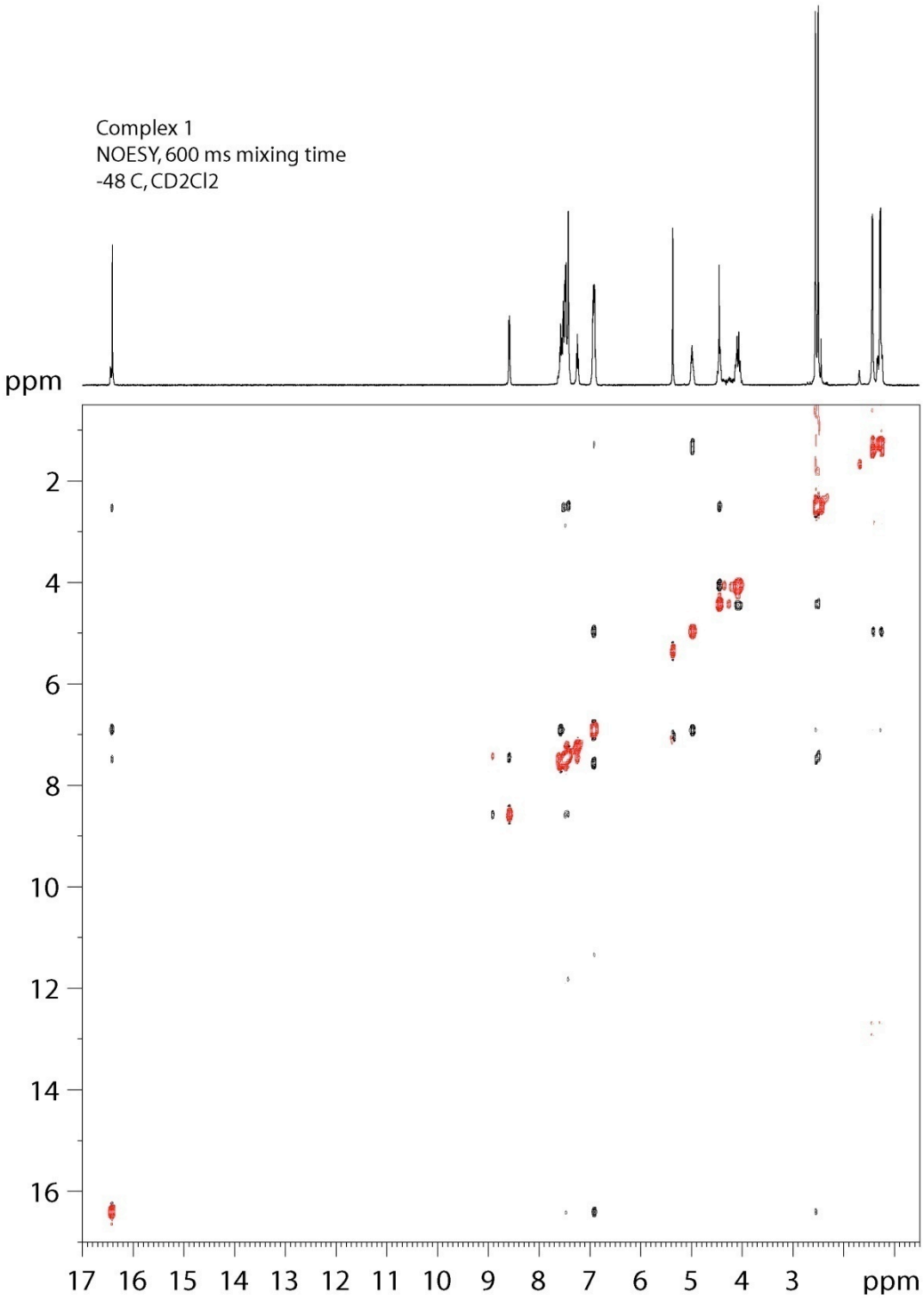


Figure S2. 400 MHz ^{1}H NOESY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2.

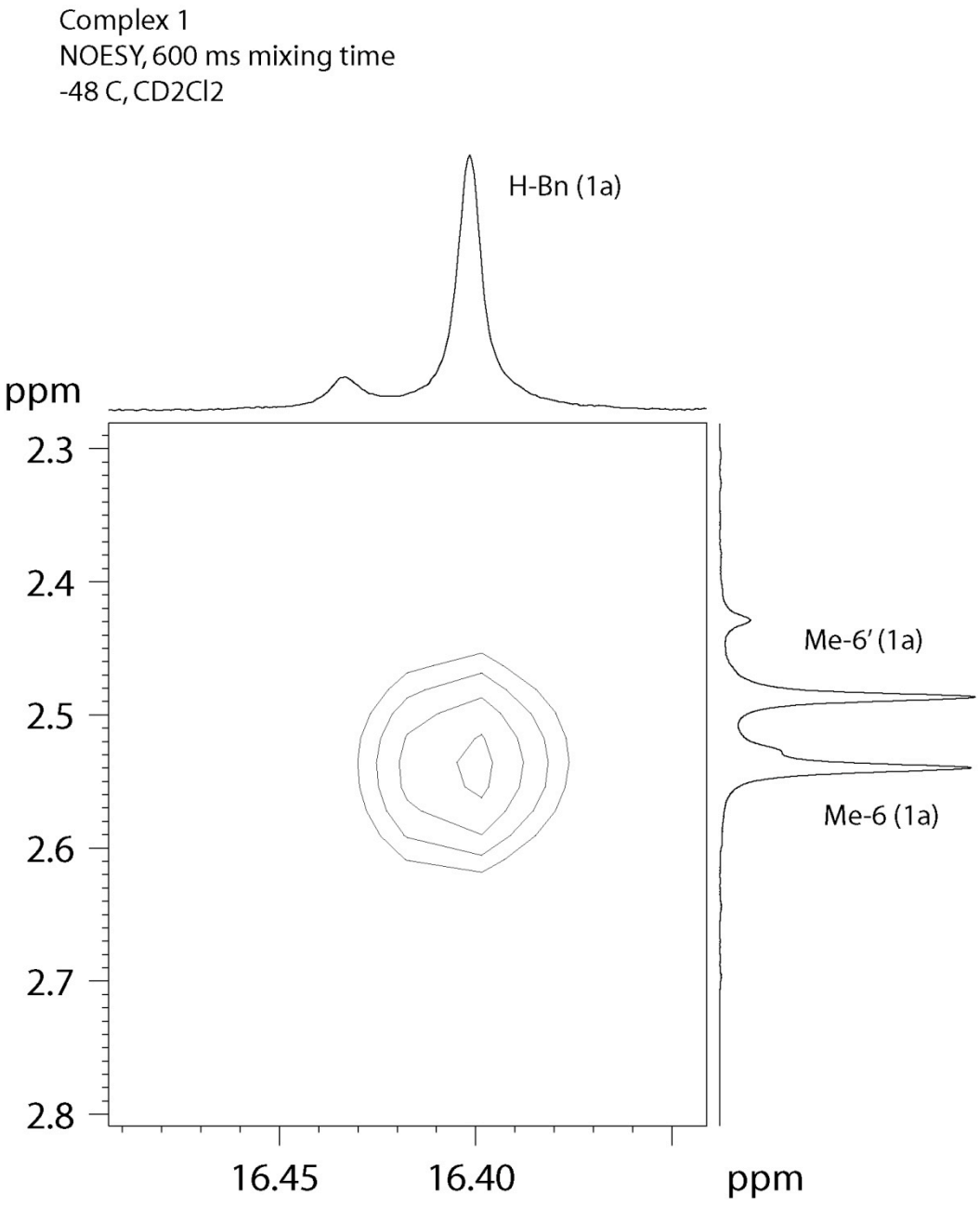


Figure S3. 400 MHz ^{1}H NOESY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2. Expansion plot showing NOE between H-Bn and Me-6.

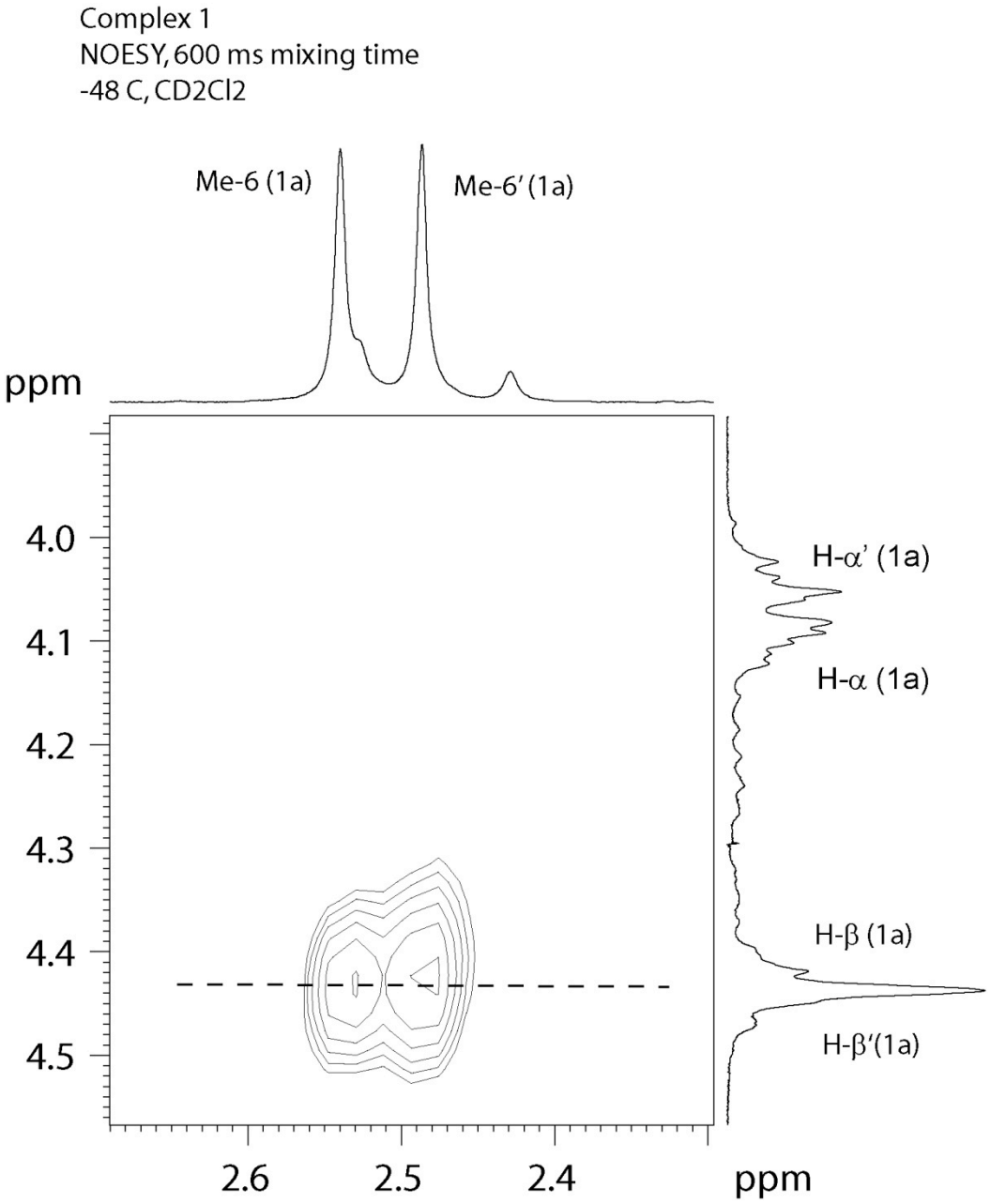


Figure S4. 400 MHz ^{1}H NOESY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2. Expansion plot showing NOEs between Me-6 and Me-6' and H-β and Hβ', respectively.

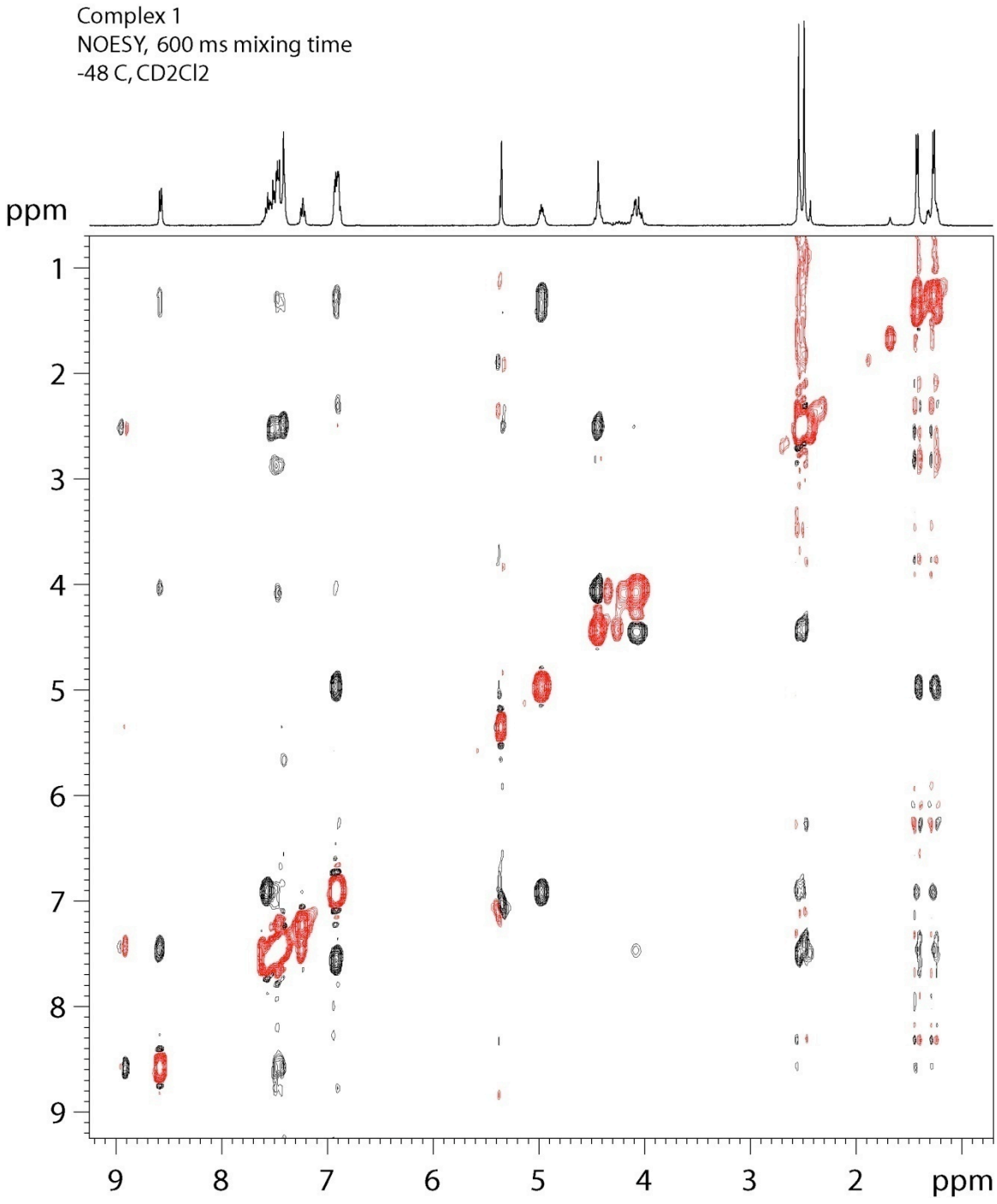


Figure S5. 400 MHz ^{1}H NOESY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2. Expansion plot showing region from 9-1 ppm.

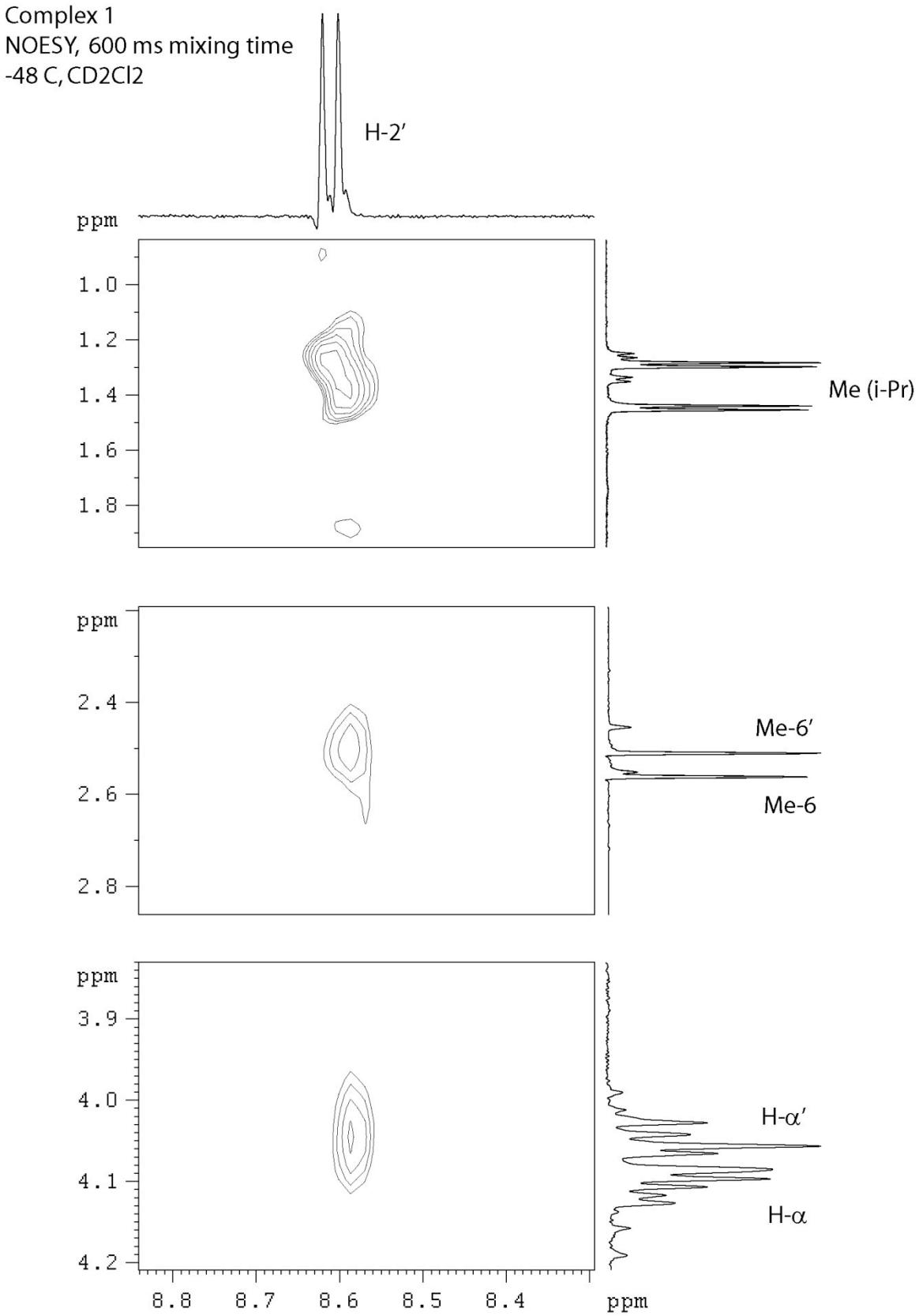


Figure S6. 400 MHz ^{1}H NOESY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2. Expansion plot showing H-2' NOEs.

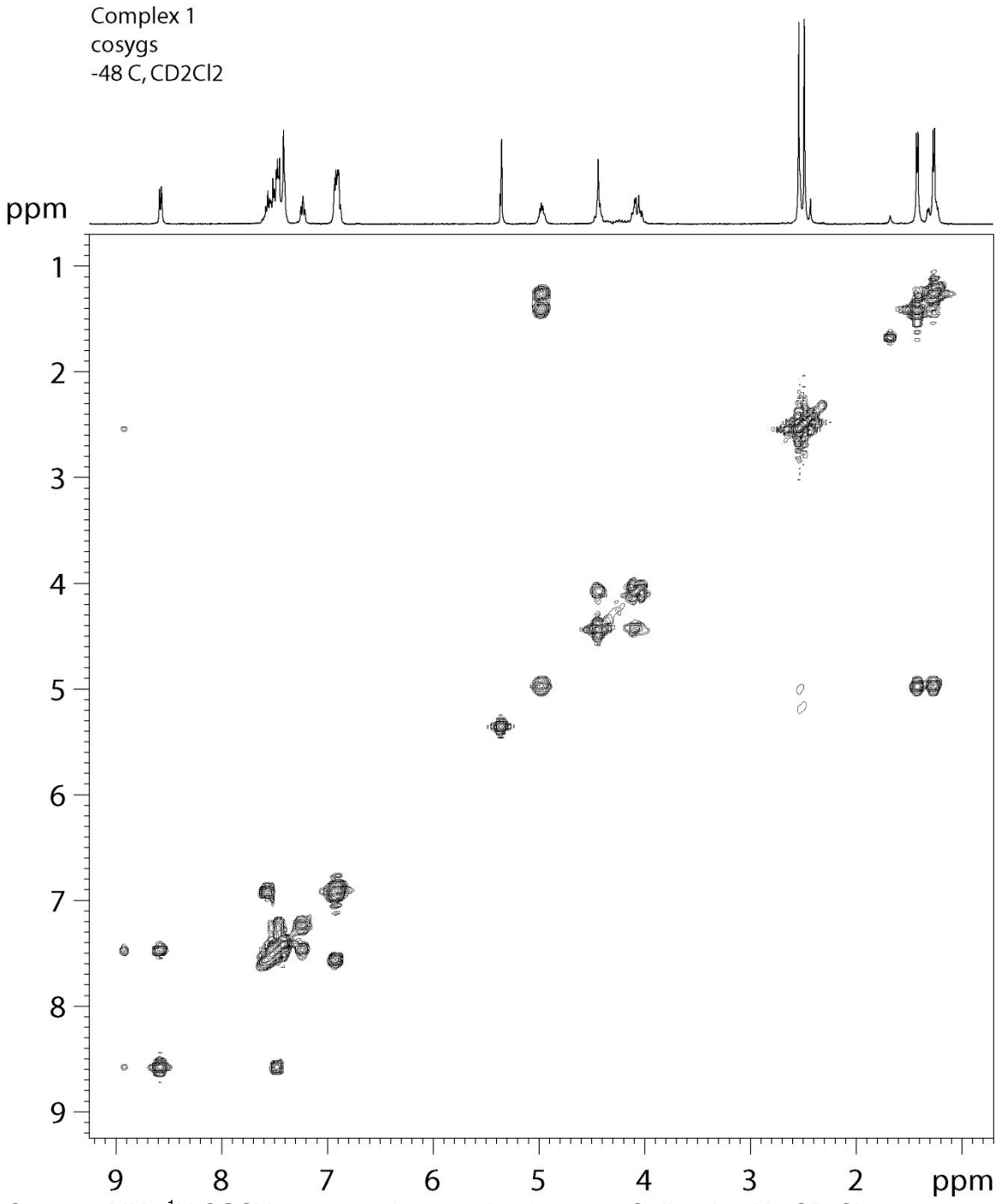


Figure S7. 400 MHz ^{1}H COSY spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2.

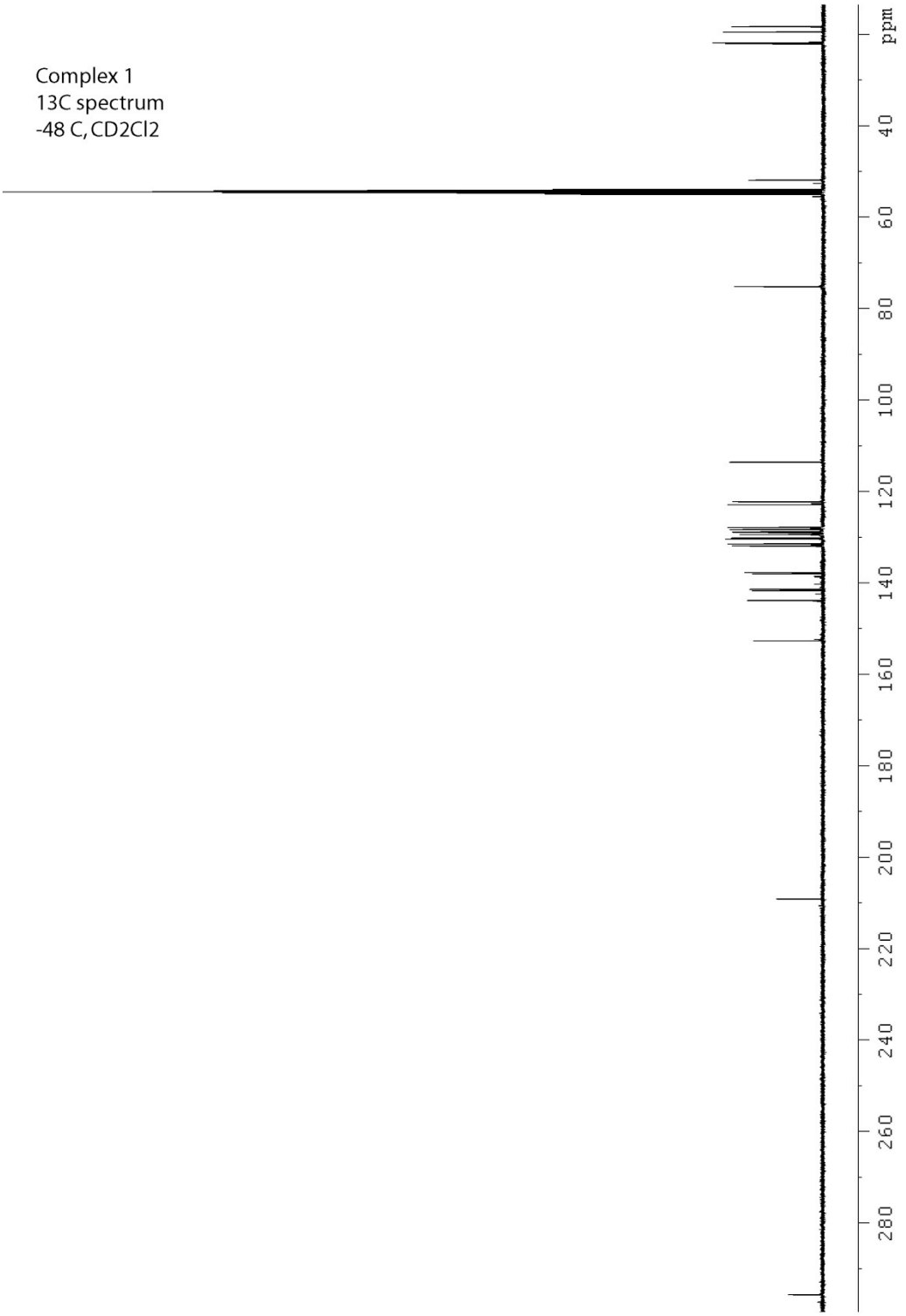


Figure S8. 100 MHz ^{13}C spectrum for complex **3** at -48 °C dissolved in CD_2Cl_2.

NMR Analysis of Olefin Complex 5

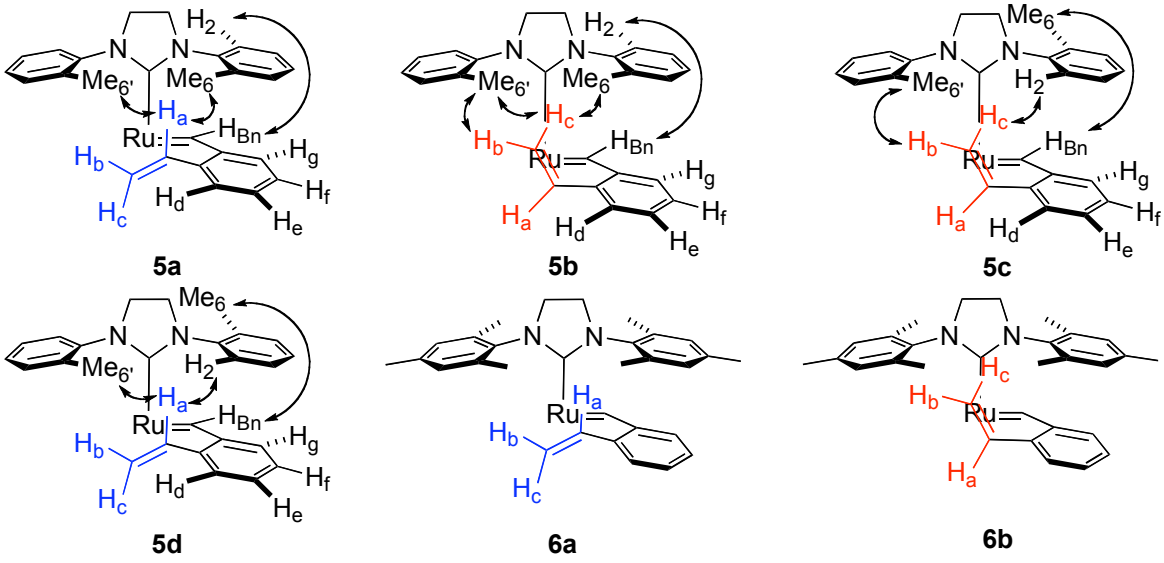


Figure S9. Naming scheme for ^{1}H NMR resonances in complexes **5** and **6**. Observed NOEs are indicated with double-headed arrows. Color has been used to clarify the geometry of the bound olefin (blue: side-bound, CH_2 down; red: side-bound, CH_2 up). Chloride ligands are omitted for clarity.

400 MHz ^{1}H selected shifts and assignments for major isomer **5a** (CD_2Cl_2, –82 °C): 15.86 ppm (1H, s, H-Bn), 8.53 (1H, d, J = 6.8 Hz, H-2'), 7.91 (1H, d, J = 8.0 Hz, H-2), 7.25 (H-3 via COSY), 7.13 (1H, t, J = 7.4 Hz), 7.00 (1H, t, J = 7.4 Hz), 6.55 (1H, d, J = 7.9 Hz), 6.37 (1H, d, J = 7.9 Hz, H-g), 4.89 (1H, dd, *J* = 12.0, 9.0 Hz, H-a), 2.55 (3H, s, Me-6'), 2.05 (1H, d, *J* = 9.0 Hz, H-b), 2.83 (1H, d, *J* = 12.0 Hz, H-c), 1.42 (3H, s, Me-6).

400 MHz ^{1}H selected shifts and assignments for second-most populated isomer **5b** (CD_2Cl_2, –82 °C): 15.40 ppm (1H, s, H-Bn), 8.66 (1H, d, J = 7.8 Hz, H-2'), 8.10 (1H, d, J = 7.3 Hz), 7.54 (H-3 via COSY), 7.43 (H-5' via NOESY), 7.02 (H-5 via NOESY), 6.37 (H-g via NOESY), 5.71 (dd, *J* = 11.8, 10.0 Hz, H-a), 2.98 (d, J = 10.0 Hz, H-b), 2.92 (d, J = 11.8 Hz, H-c), 2.39 (3H, s, Me-6'), 1.17 (3H, s, Me-6).

400 MHz ^{1}H selected shifts and assignments for third-most populated isomer **5c** (CD_2Cl_2, –82 °C): 15.32 ppm (1H, s, H-Bn), 8.75 (1H, d, J = 7.8 Hz, H-2'), 7.52 (H-5 via NOESY), 7.38 (H-4 via NOESY), 6.71 (H-3 via NOESY), 6.01 (1H, d, J = 7.6 Hz, H-2), 5.76 (dd, J = 10, 12 Hz, Ha), 2.905 (3H, s, Me-6), 2.83 (d, J = 10 Hz, Hb), 2.59 ppm (d, J = 12 Hz, Hc), 2.375 (3H, s, Me-6').

400 MHz ^{1}H selected shifts and assignments for fourth-most populated isomer **5d** (CD_2Cl_2, –82 °C): 16.01 ppm (1H, s, H-Bn), 7.235 (H-5 via NOESY), 7.08 (H-4 via NOESY), 6.22 (H-3 via NOESY), 5.61 (d, J = 7.6 Hz, H-2), 5.10 (dd, J = 10, 12 Hz, H-a), 3.03 (d, J = 12 Hz, H-c), 2.546 (3H, s, Me-6/6'), 2.03 (d, J = 10 Hz, H-b).

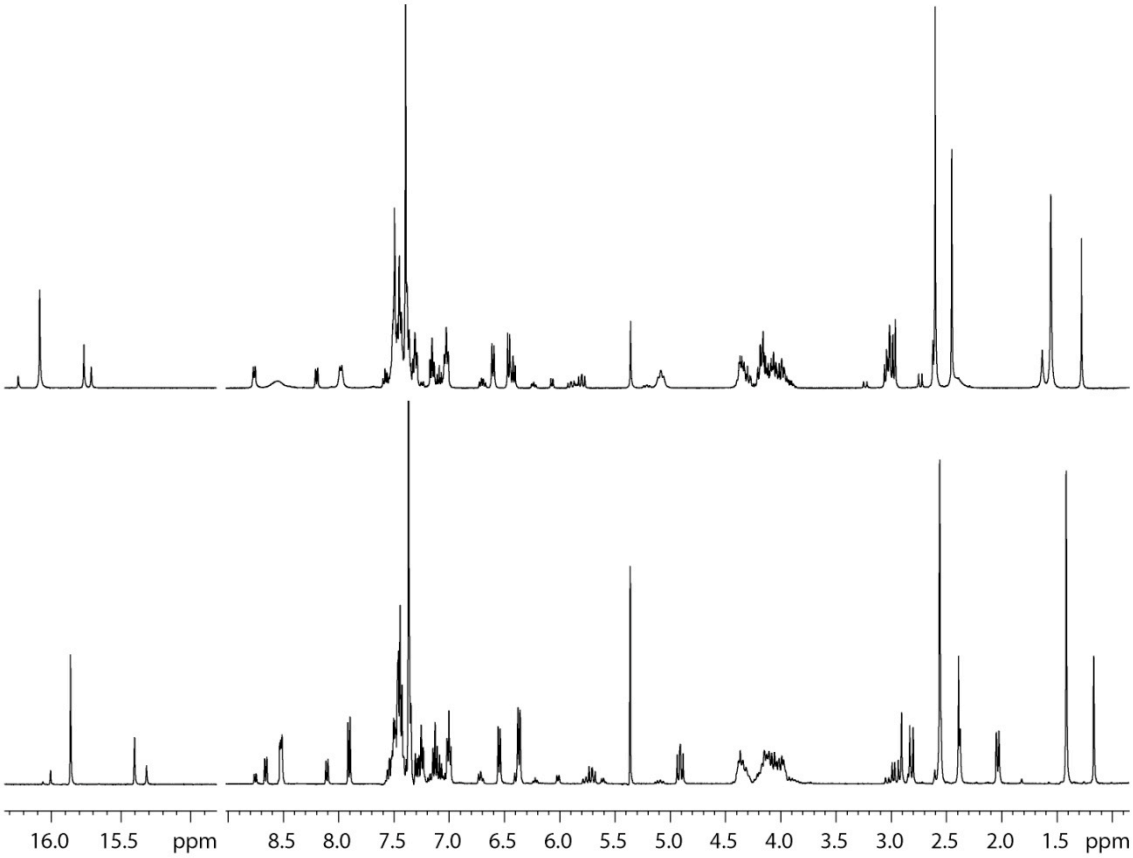


Figure S10. 400 MHz ^{1}H spectrum of complex **5** dissolved in CD_2Cl_2. Top: spectrum recorded at 19 °C. Bottom: spectrum recorded at –82 °C.

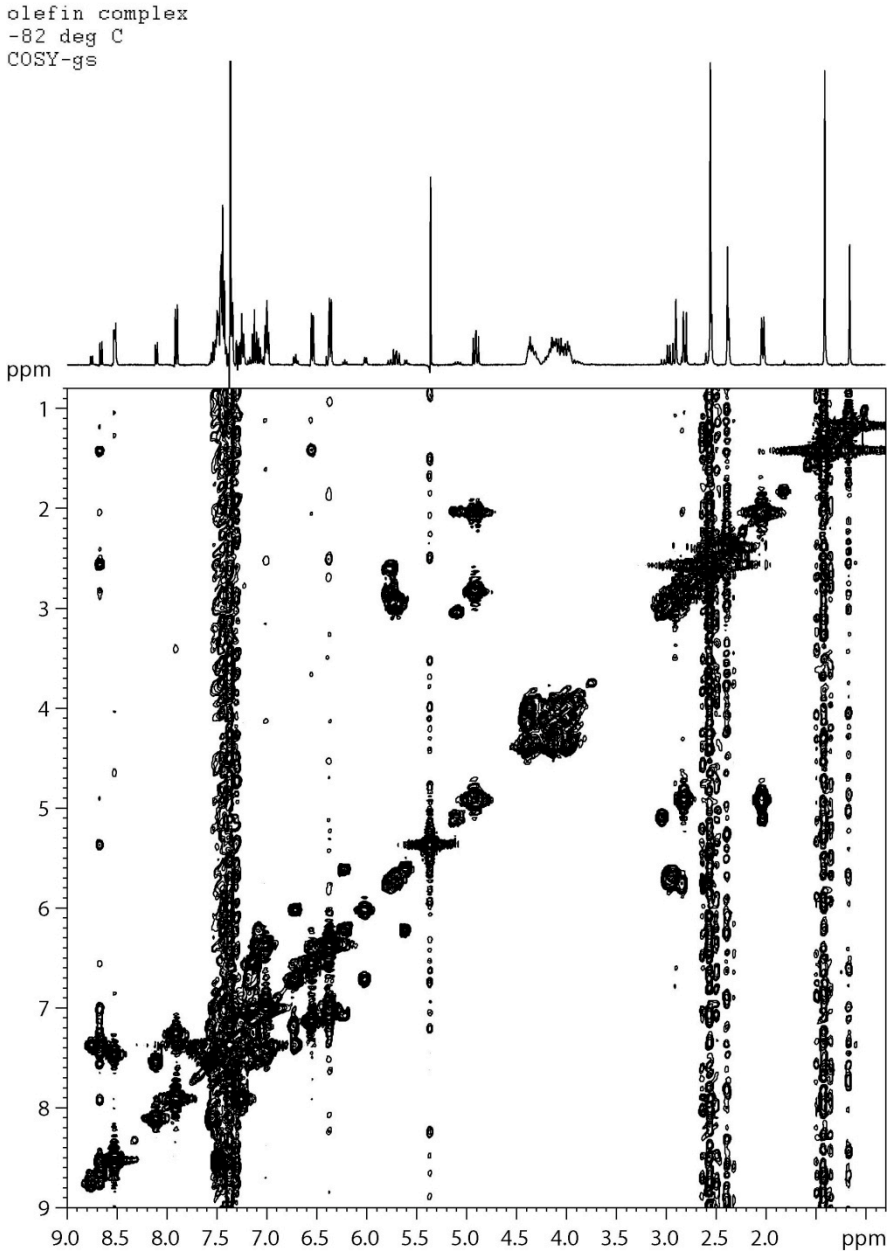


Figure S11. 400 MHz ^{1}H COSY spectrum for complex **5** at -82 °C dissolved in CD_2Cl_2.

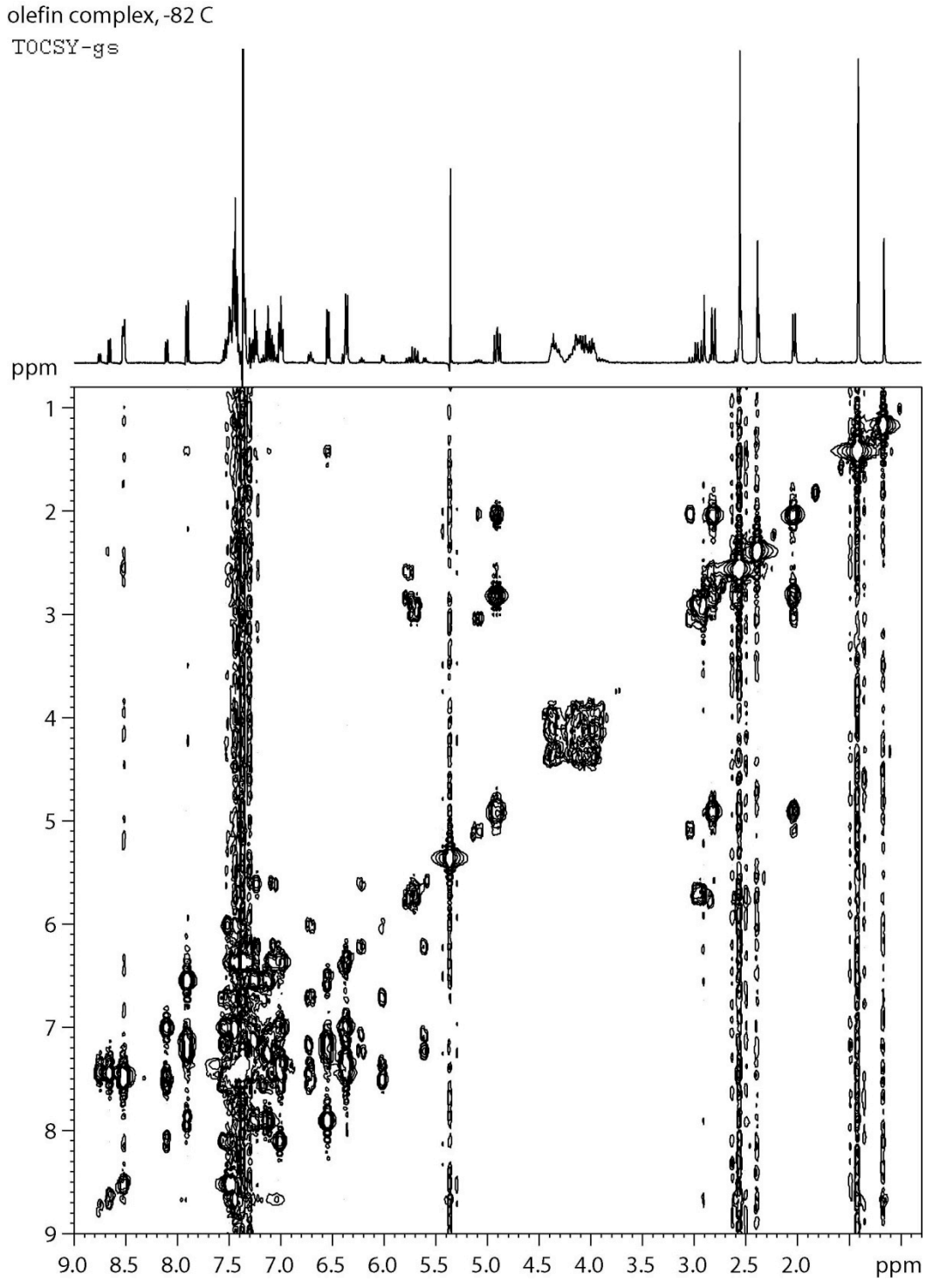


Figure S12. 400 MHz ^{1}H TOCSY spectrum for complex **5** at -82 °C dissolved in CD_2Cl_2.

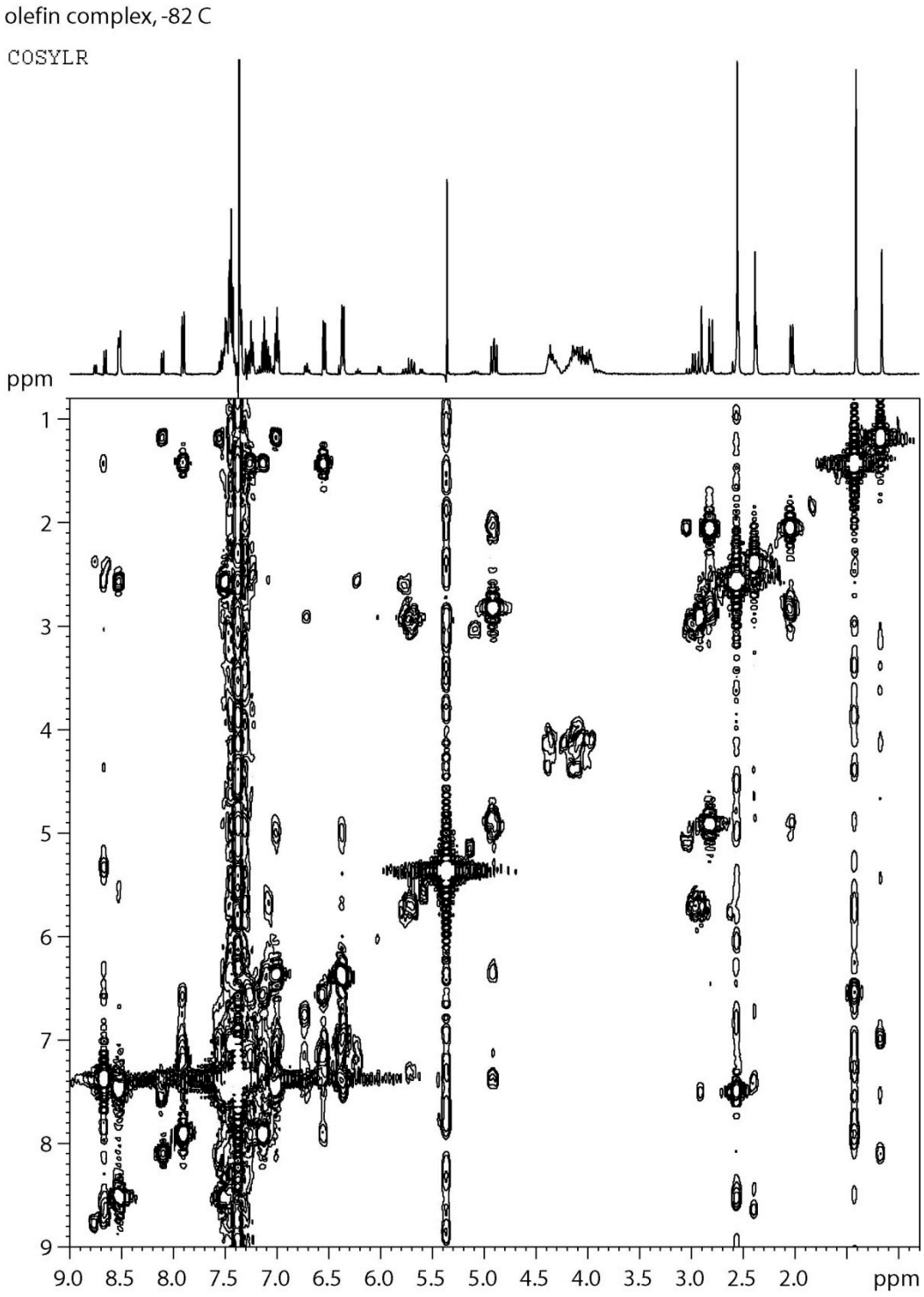


Figure S13. 400 MHz ^{1}H COSY-LR spectrum for complex **5** at -82 °C dissolved in CD_2Cl_2.

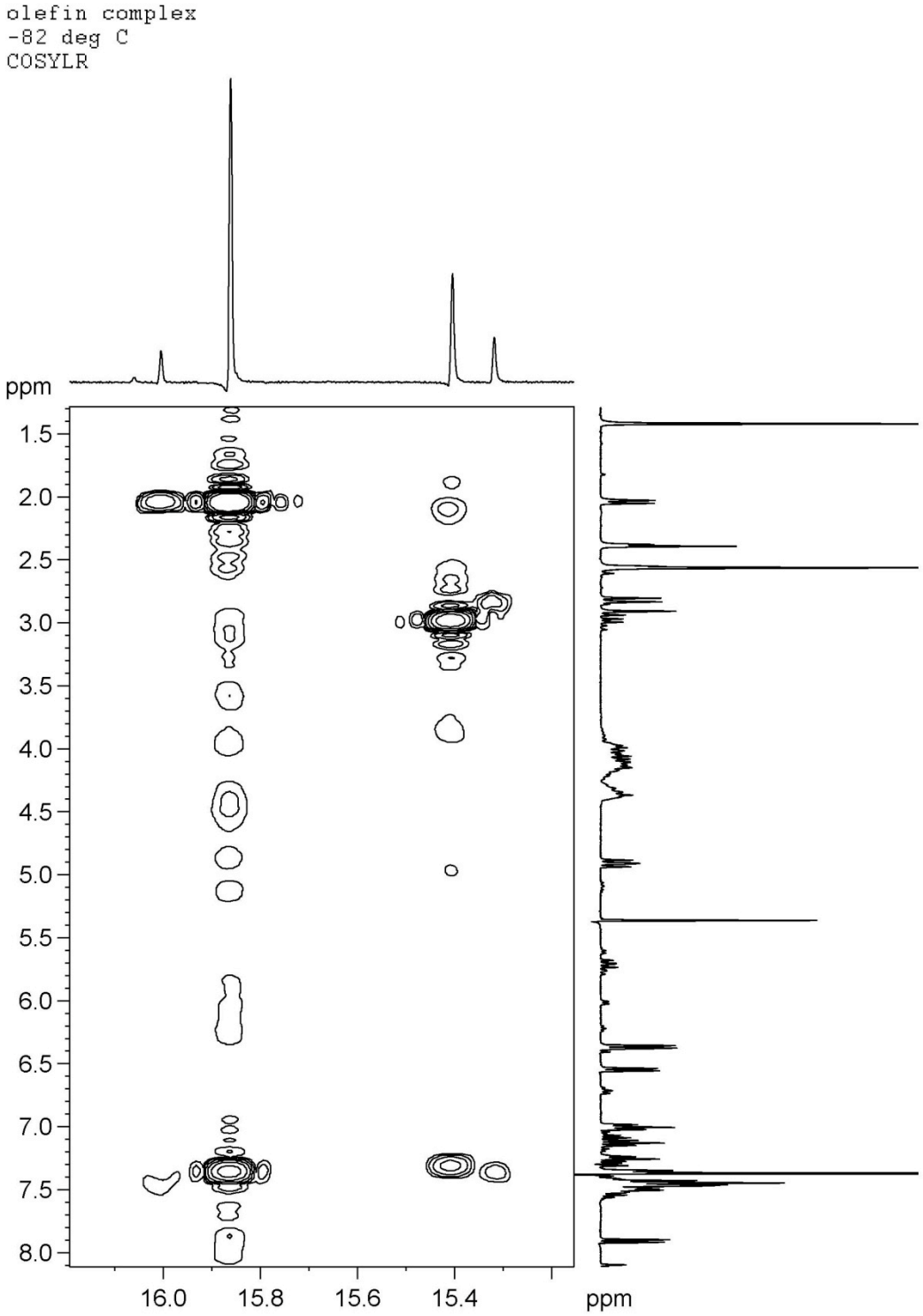


Figure S14. 400 MHz ^{1}H COSY-LR spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD_2Cl_2.

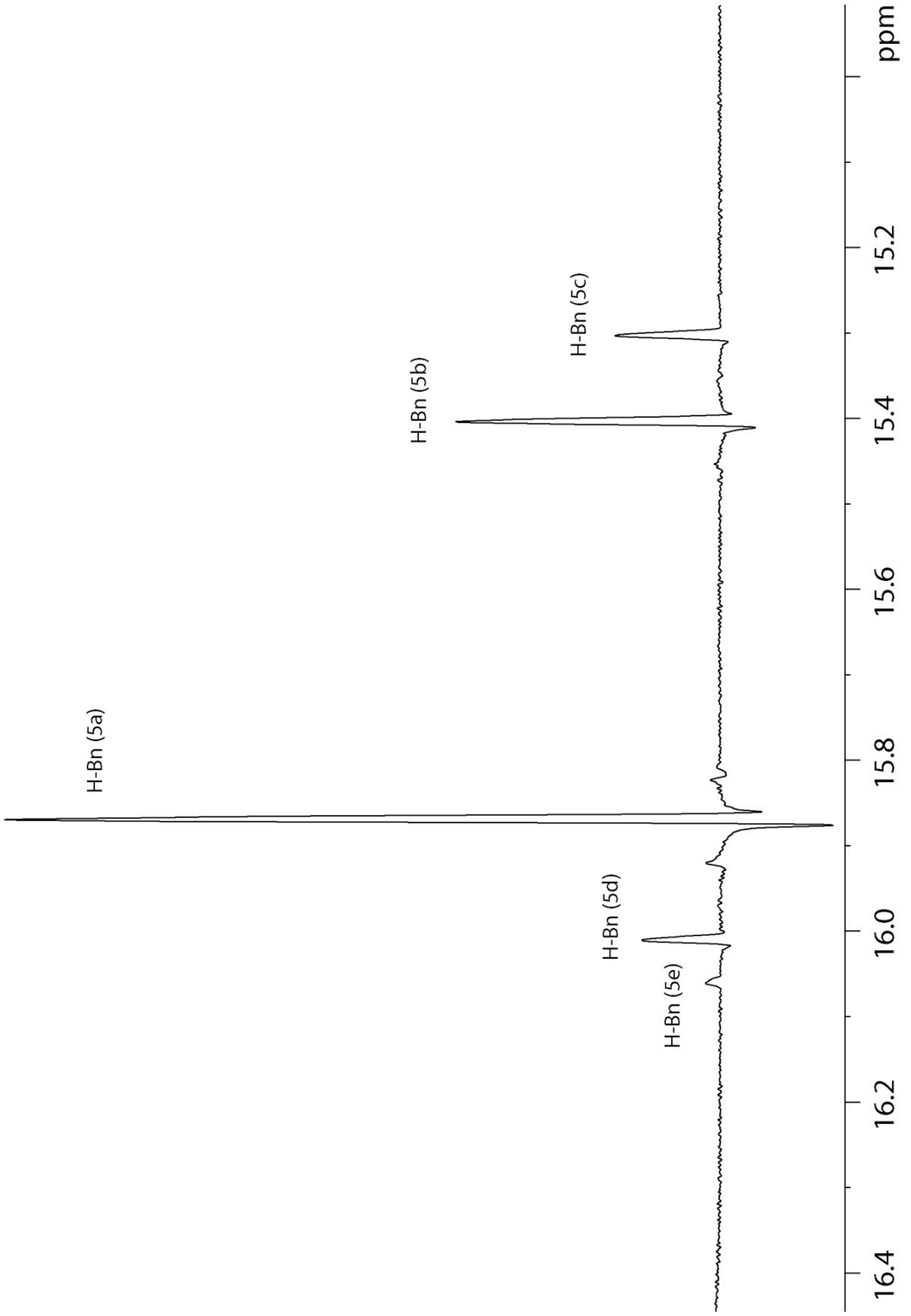


Figure S15. 400 MHz ^{1}H spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD_2Cl_2.

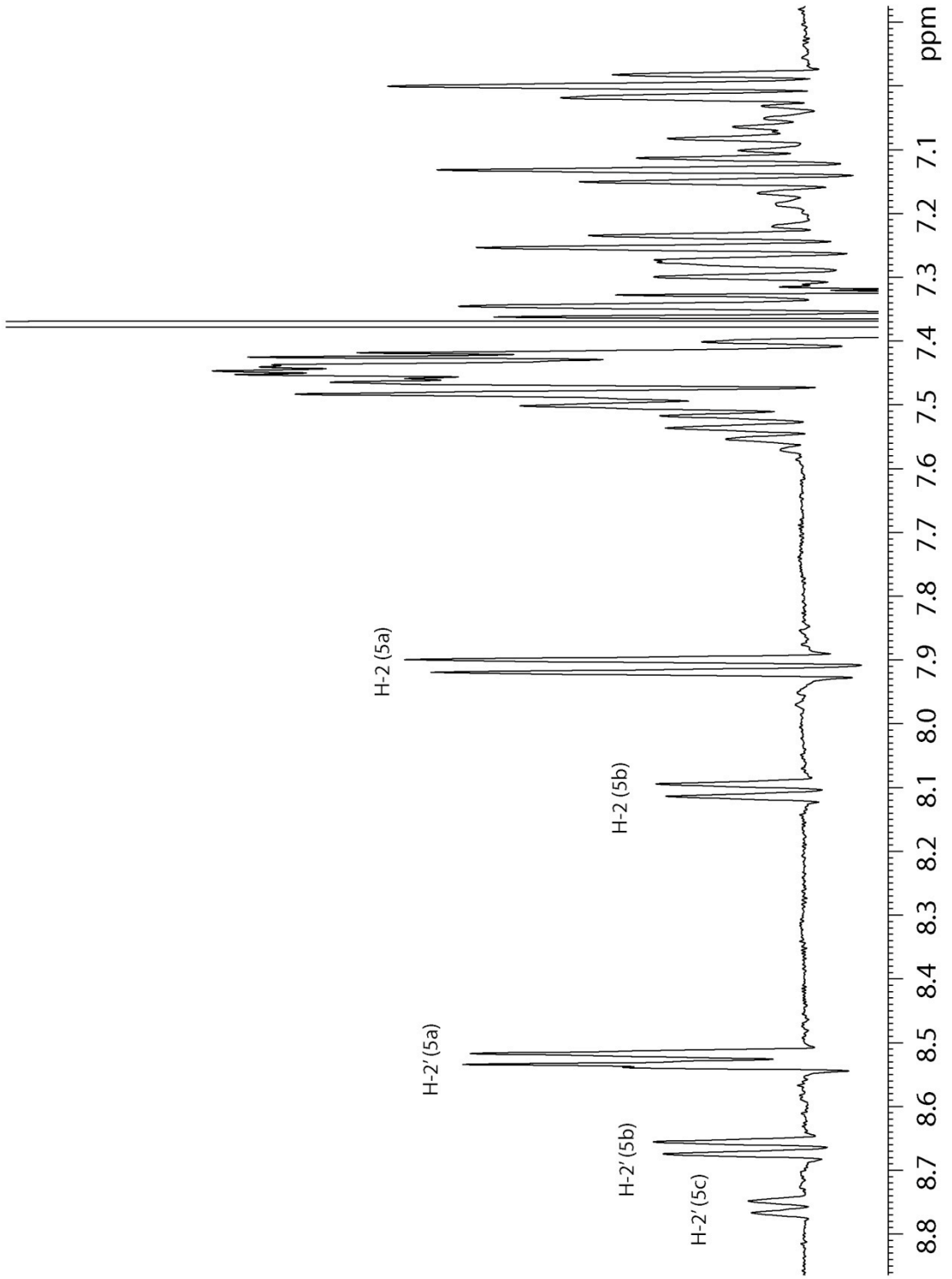


Figure S16. 400 MHz ^{1}H spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD_2Cl_2.

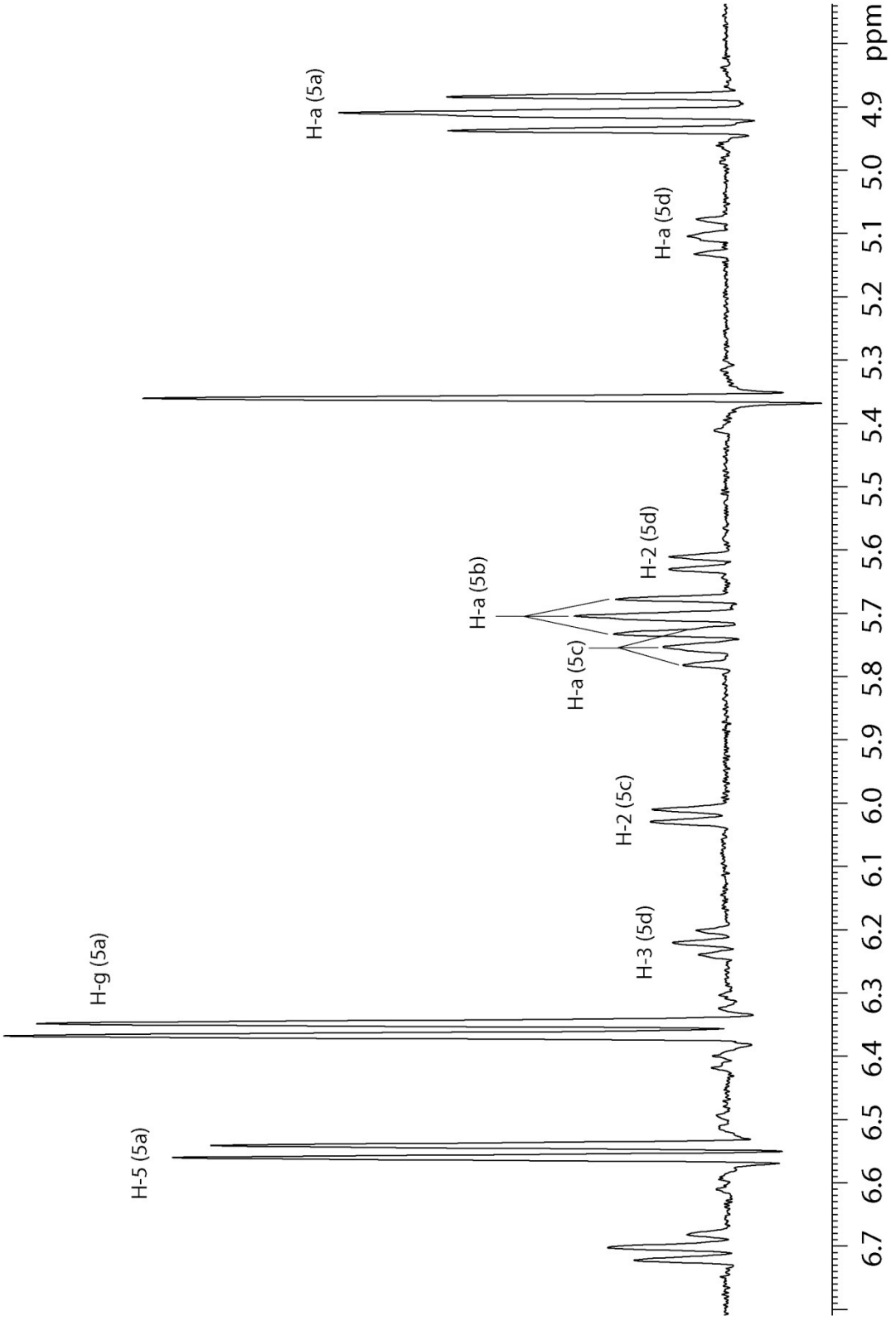


Figure S17. 400 MHz ^{1}H spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD_2Cl_2.

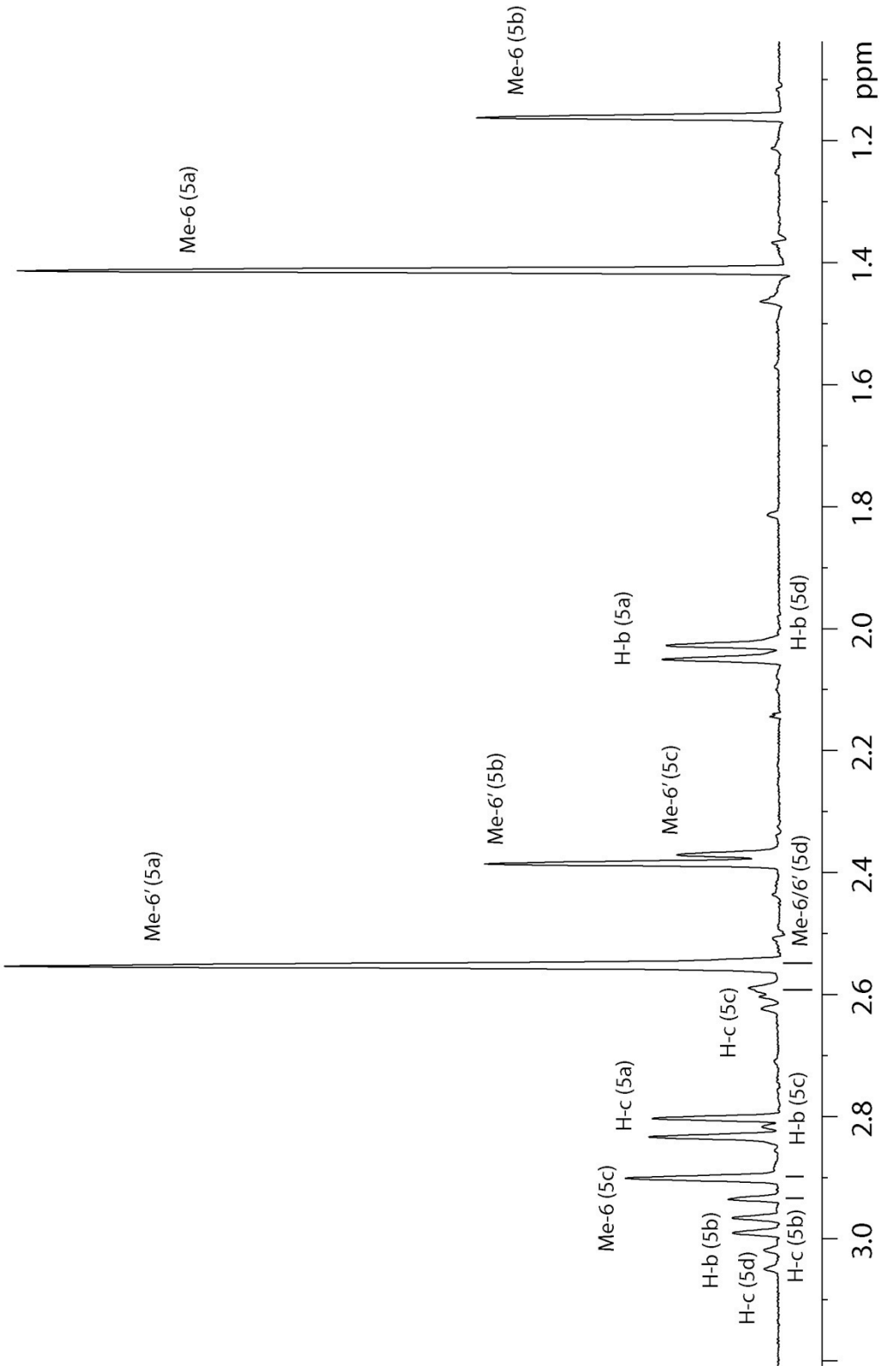


Figure S18. 400 MHz ^{1}H spectrum (expansion plot) for complex **5** at -82 °C dissolved in CD_2Cl_2.

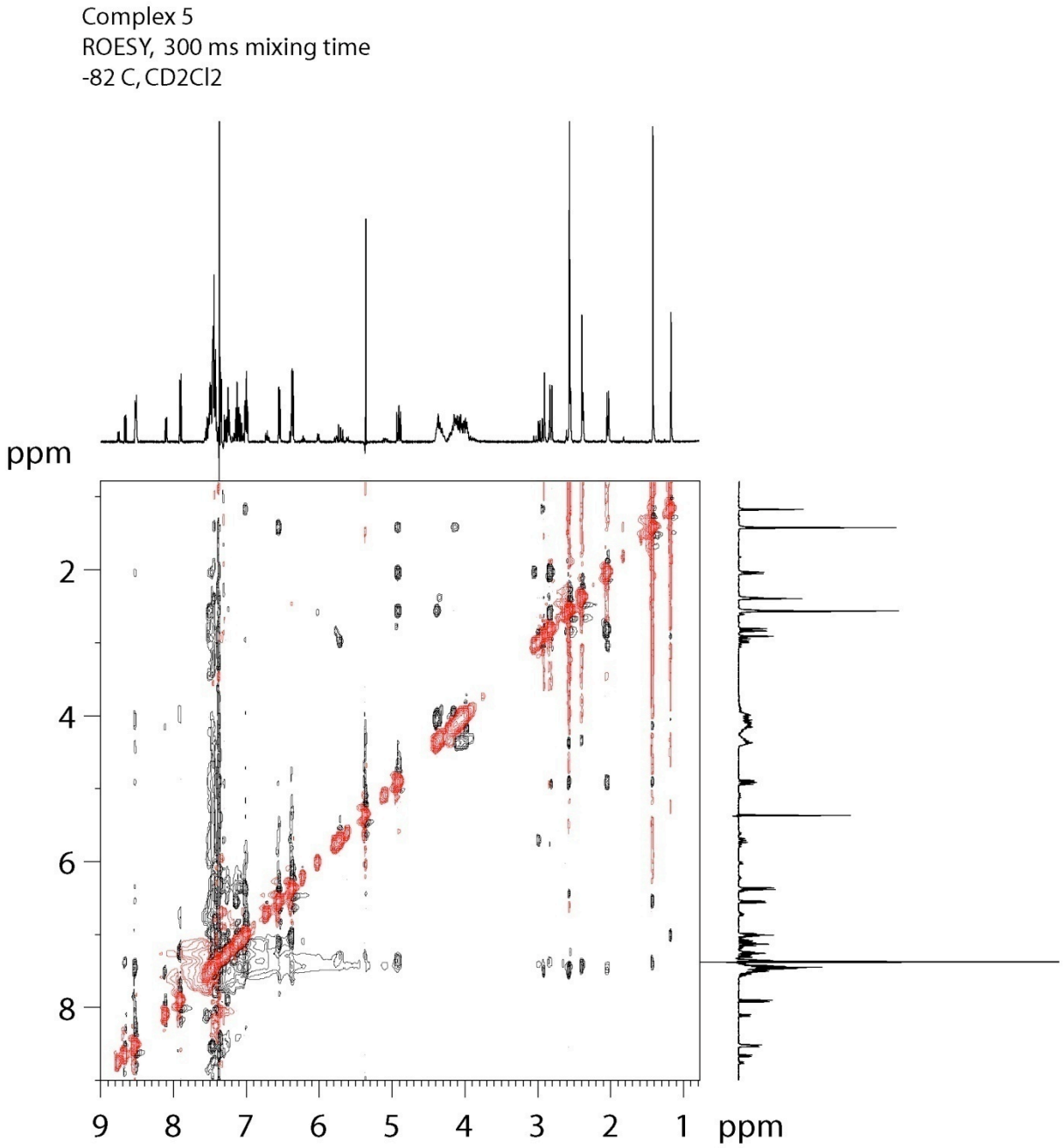


Figure S19. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

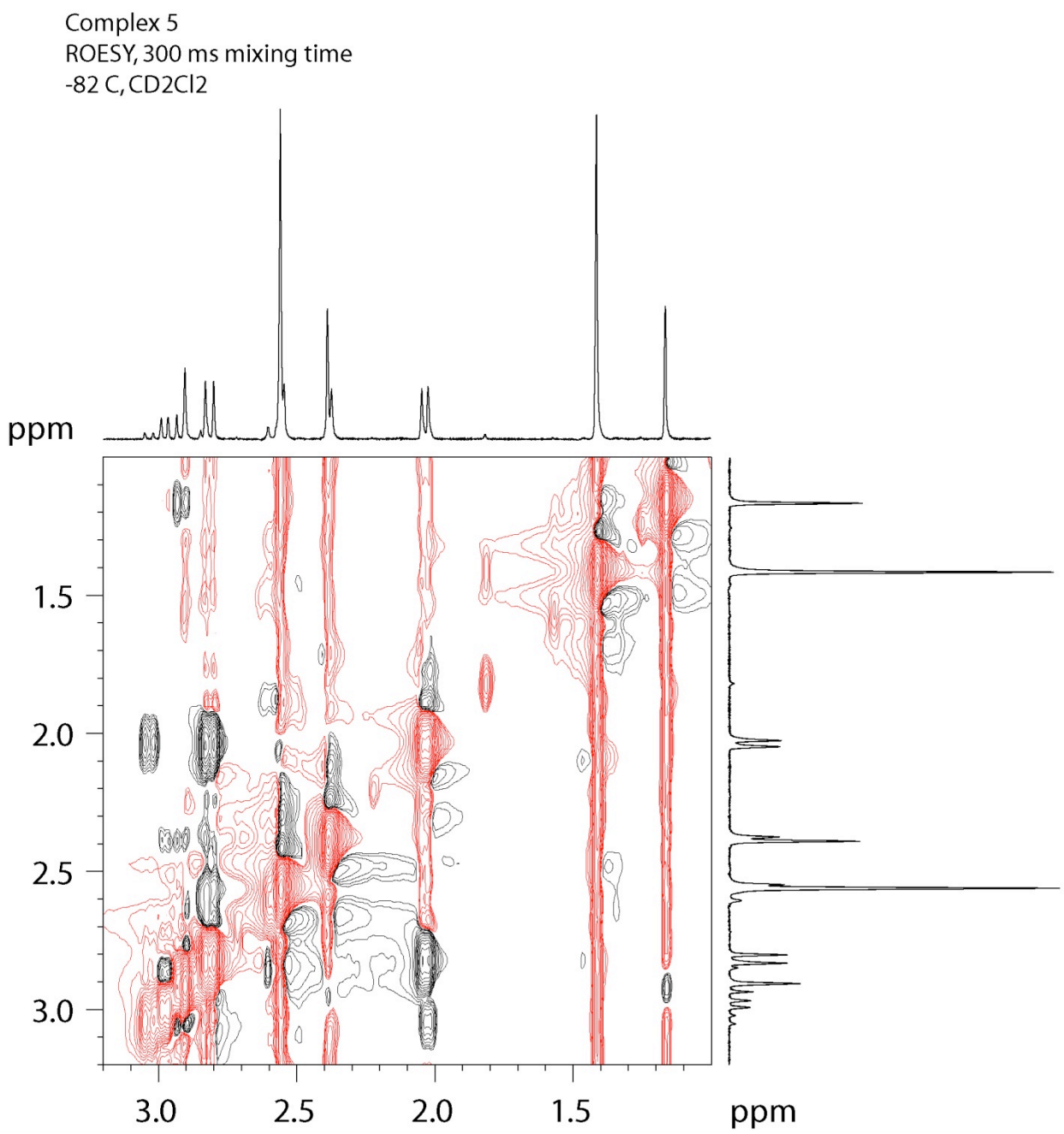


Figure S20. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

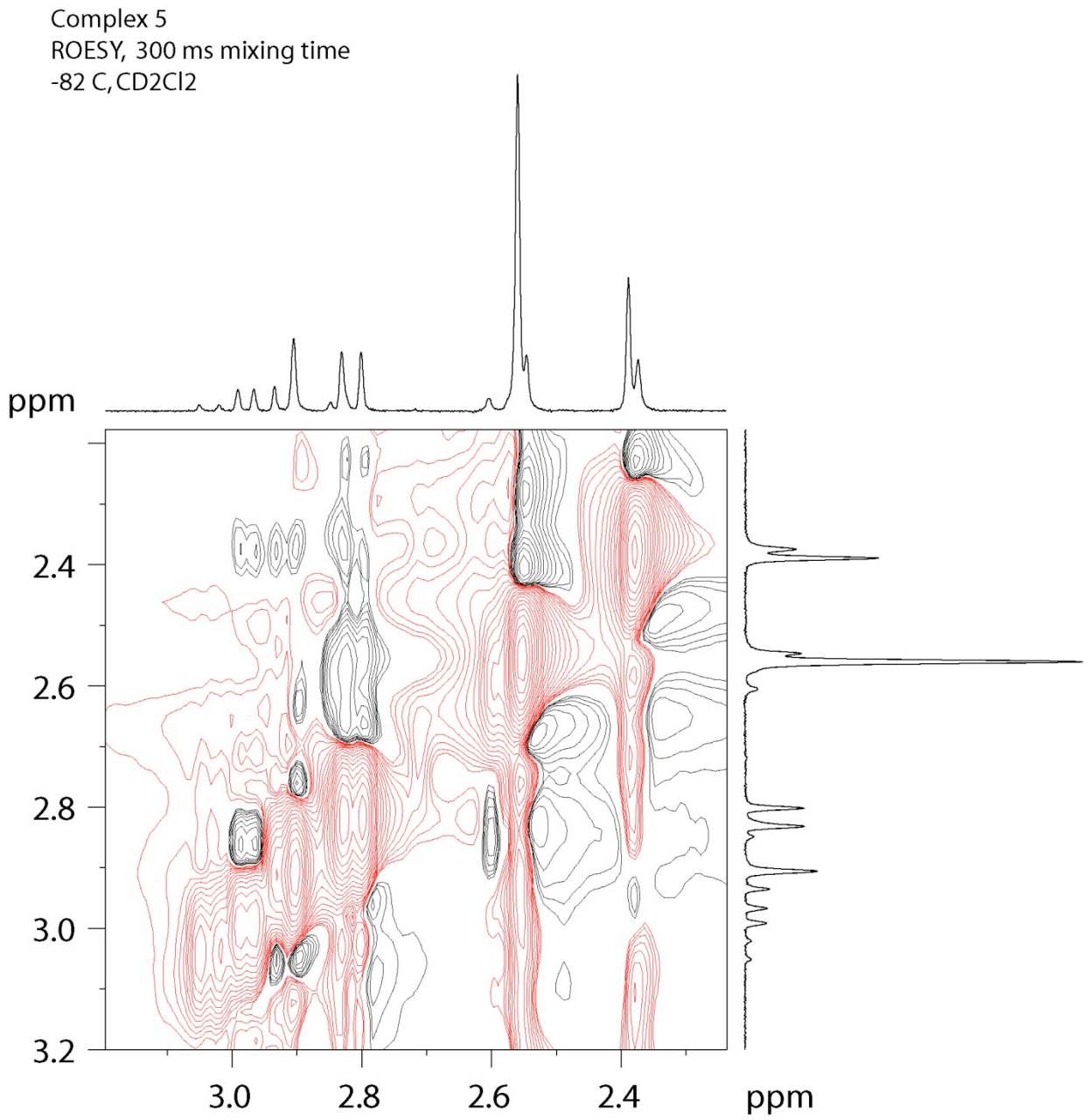


Figure S21. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

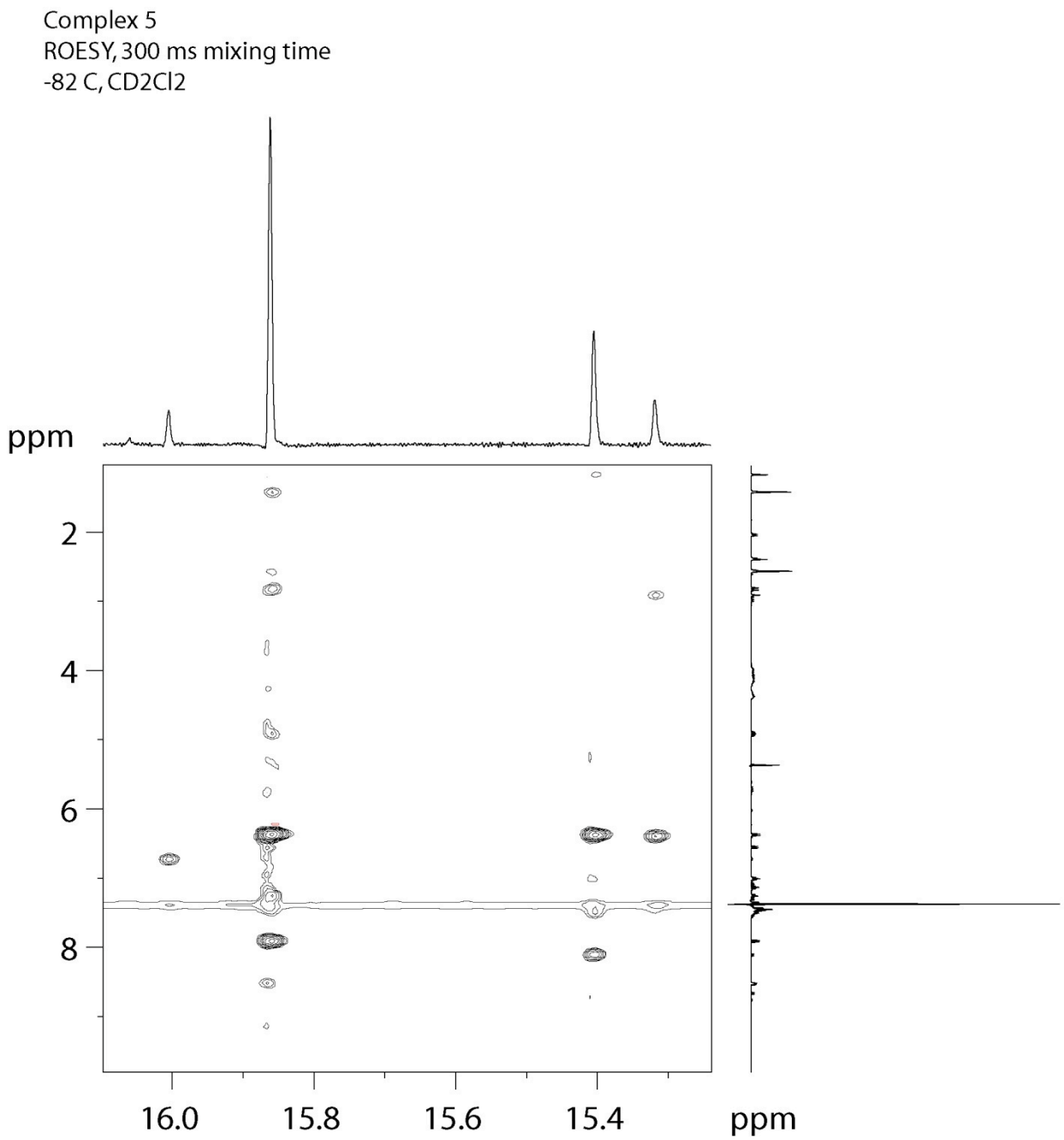


Figure S22. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

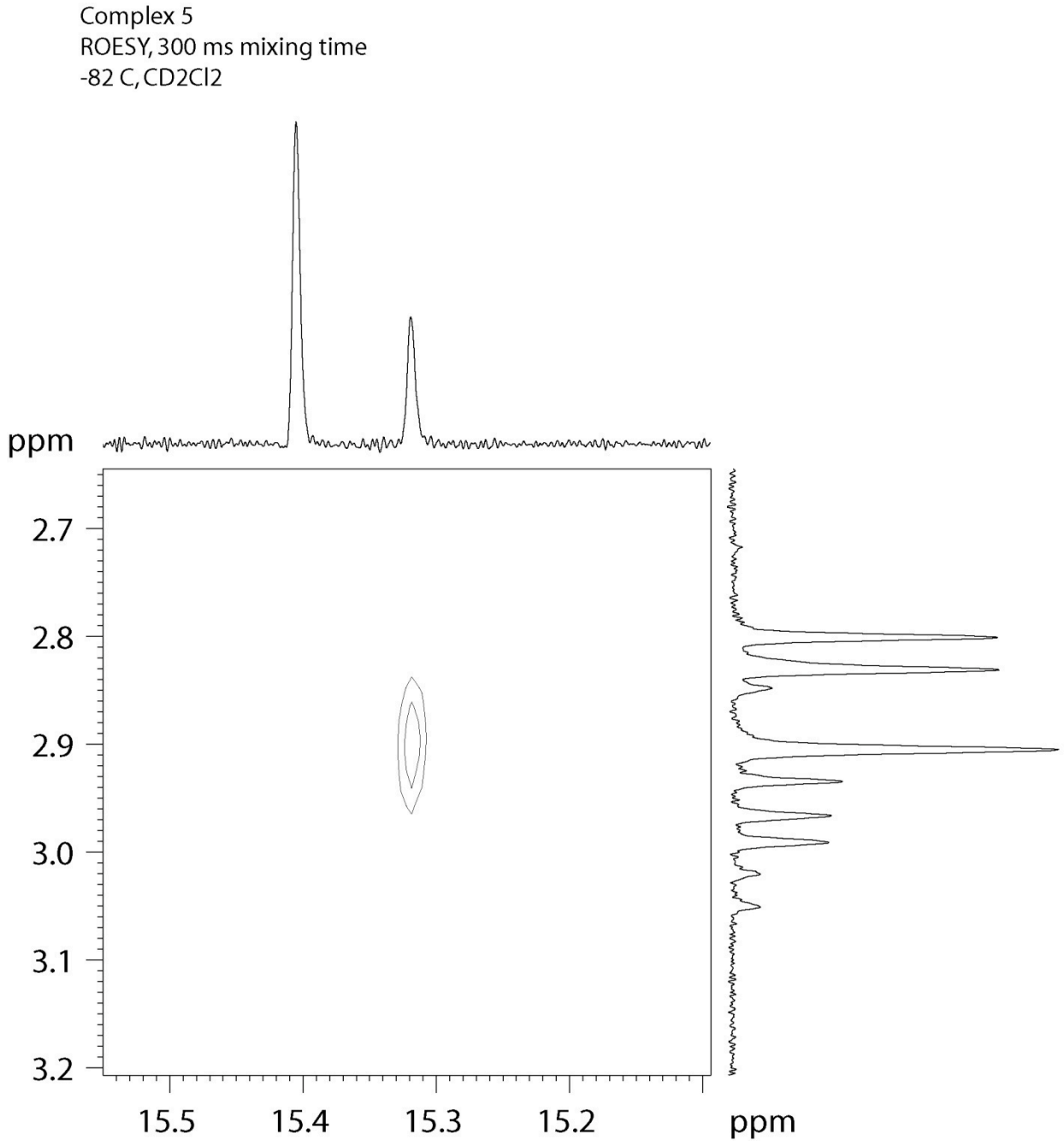


Figure S23. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

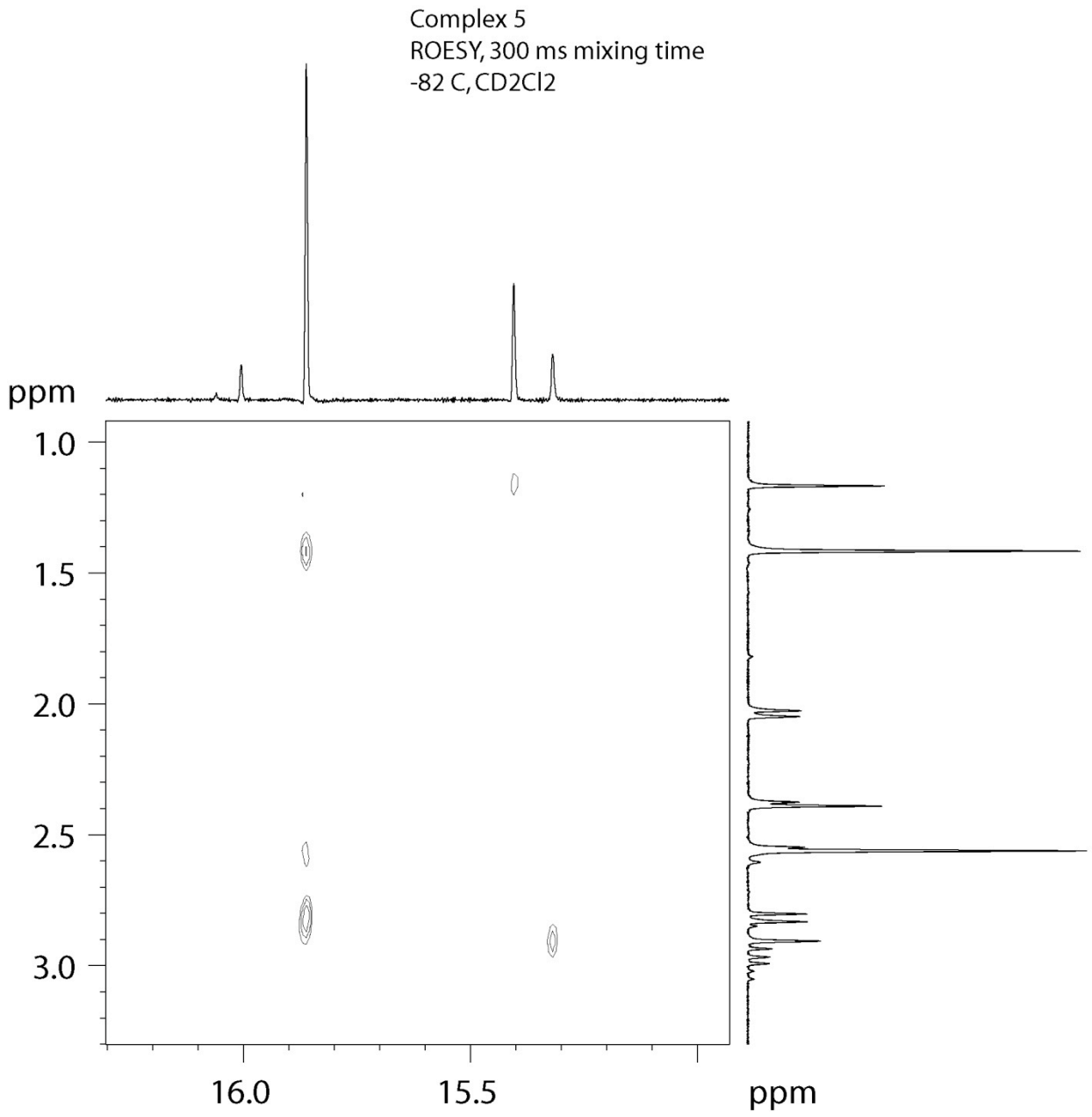


Figure S24. 400 MHz ^{1}H ROESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

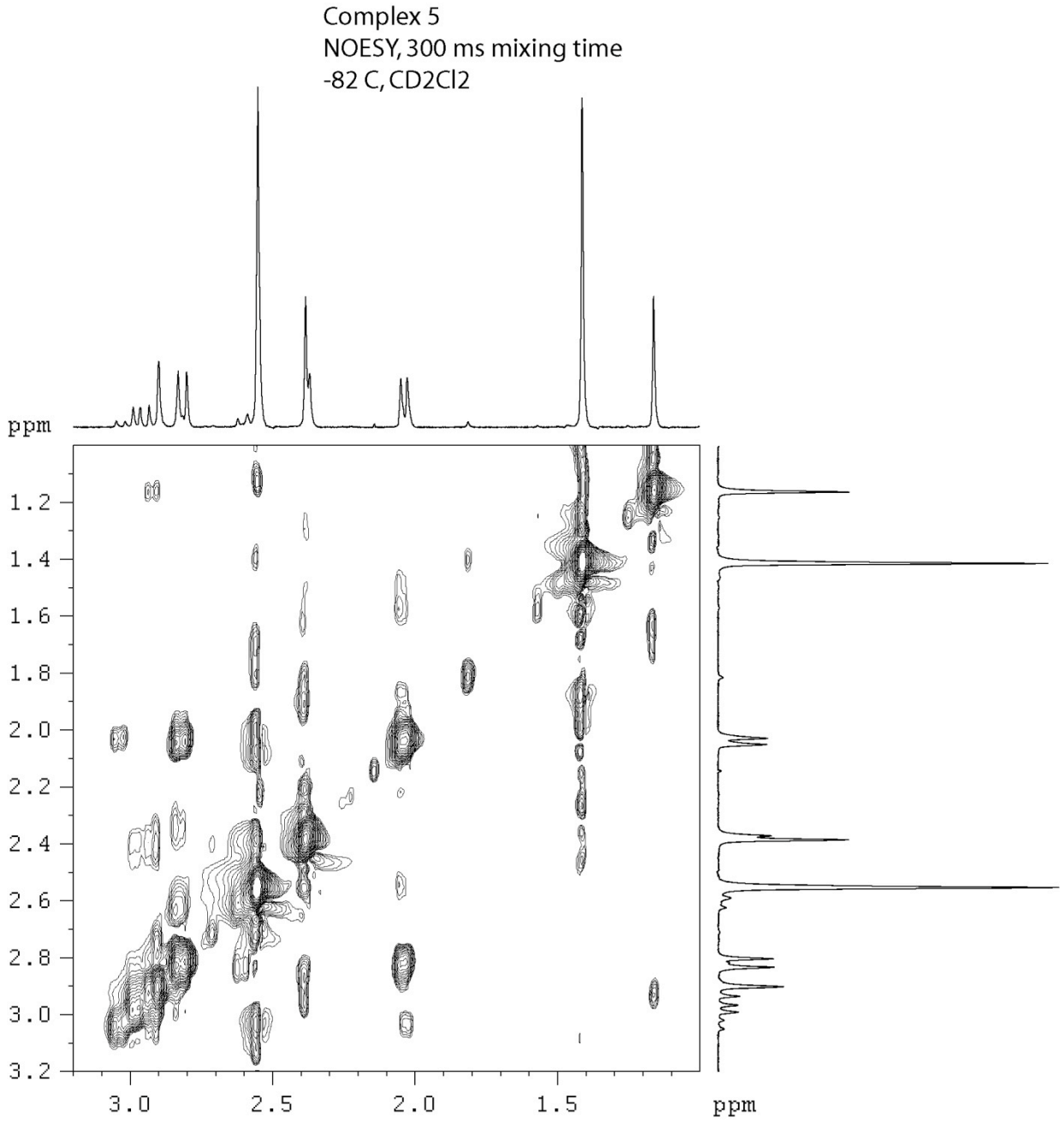


Figure S25. 400 MHz ^{1}H NOESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

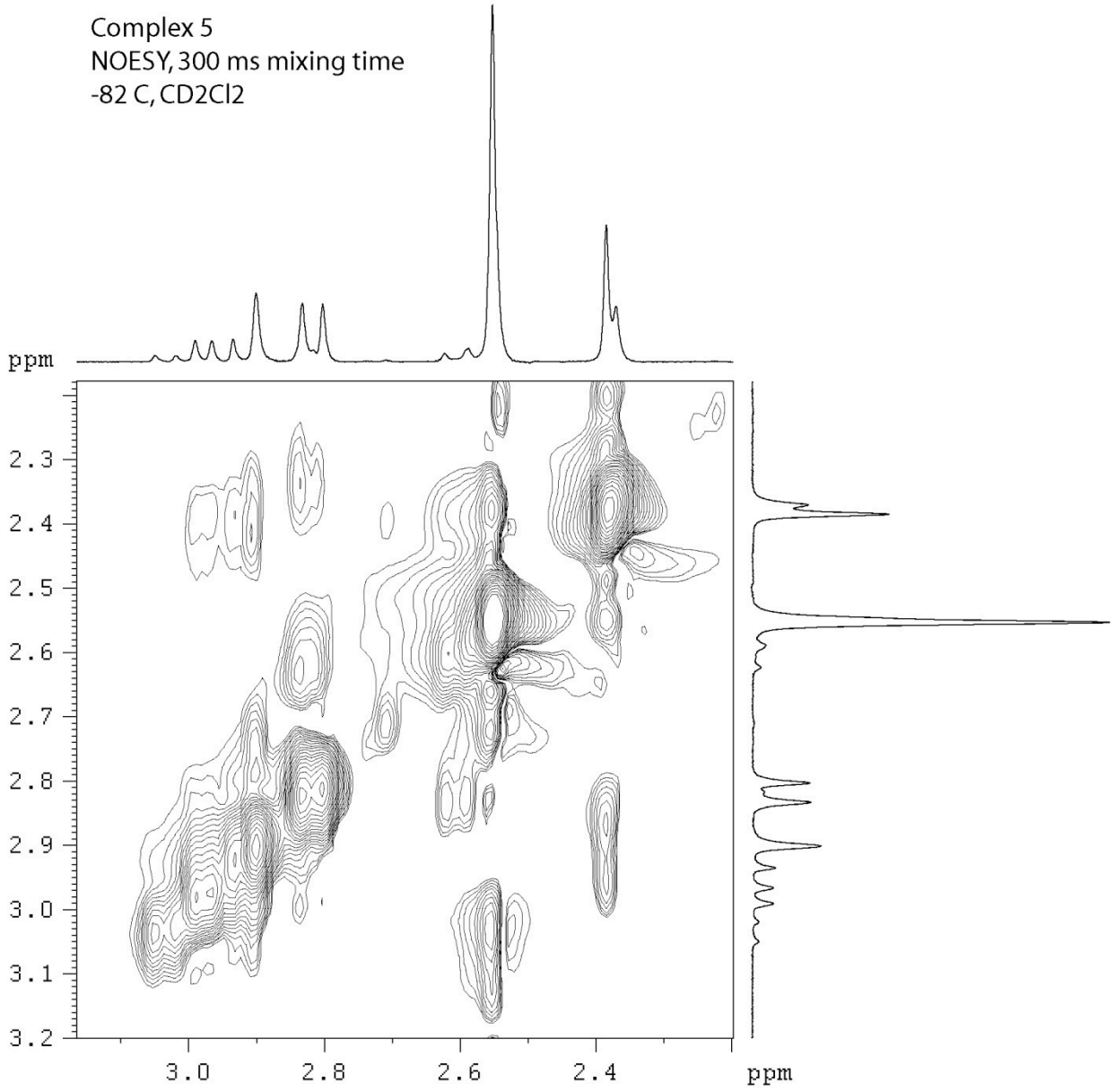


Figure S26. 400 MHz ^{1}H NOESY experiment for complex **5** at -82 °C dissolved in CD_2Cl_2.

Computational Section

V.1 Methods. Calculations were performed on all systems using density functional theory (DFT) with the B3LYP, M06 and M06-L functionals, as implemented in Jaguar 7.0 (release 207).[1] B3LYP utilizes both exact Hartree-Fock (HF) exchange and corrections (generalized gradient approximation) to the Slater exchange functional, the Becke three-parameter functional (B3) with the Becke gradient correction,[2] the Vosko-Wilk-Nusair exchange functional,[3] and the correlation functional of Lee, Yang, and Parr (LYP).[4]

The M06 functional is a new hybrid meta-GGA exchange-correlation functional that leads to impressive accuracy for a very large validation set of systems, including van der Waals dimers, reactions, and transition metal complexes. However, only a limited number of M06 tests have been reported for reactions of transition metal catalysts.

All calculations used the Hay and Wadt small core-valence relativistic effective-core-potential[5] (ECP) to describe the 1s-3d core electrons of the ruthenium atom, leaving the outer 16 electrons (4s, 4p, 4d, 5s, *etc*.) to be treated explicitly.

Our previous results showed that the LACVP** basis set produces geometries in good agreement with experiment and that the extended LACV3P++** basis set[6] describes properly the energy of intermediates relevant to olefin metathesis. Here LACVP** was used for all geometry optimizations and LACV3P++**(2f) for energies. LACV3P++**(2f) utilizes the LACV3P++** basis set as implemented in Jaguar plus a double-zeta f-shell with exponents reported by Martin and Sundermann.[7] All electrons were described for all other atoms using the 6-31G** or 6-311++G** basis sets.[8]

Every structure was optimized in the gas phase with the B3LYP and M06-L functionals as noted. For each B3LYP optimized structure, the analytic Hessian was calculated to obtain the vibrational frequencies, which in turn were used to obtain the zero point energies and free energy corrections (without translational or rotational components) to 298 K or as noted. Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for CH_2Cl_2 (ε = 8.93 and R_0= 2.33 Å) or benzene (ε = 2.284 and R_0= 2.60 Å) using the PBF[9] module in Jaguar, which has been shown[10] recently to give quite accurate results. (ε is dielectric constant and R_0 is the solvent's probe radius, see ref. 9 for more details)

Theoretical References

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Electronic Energies, Solvation and Thermodynamic Corrections

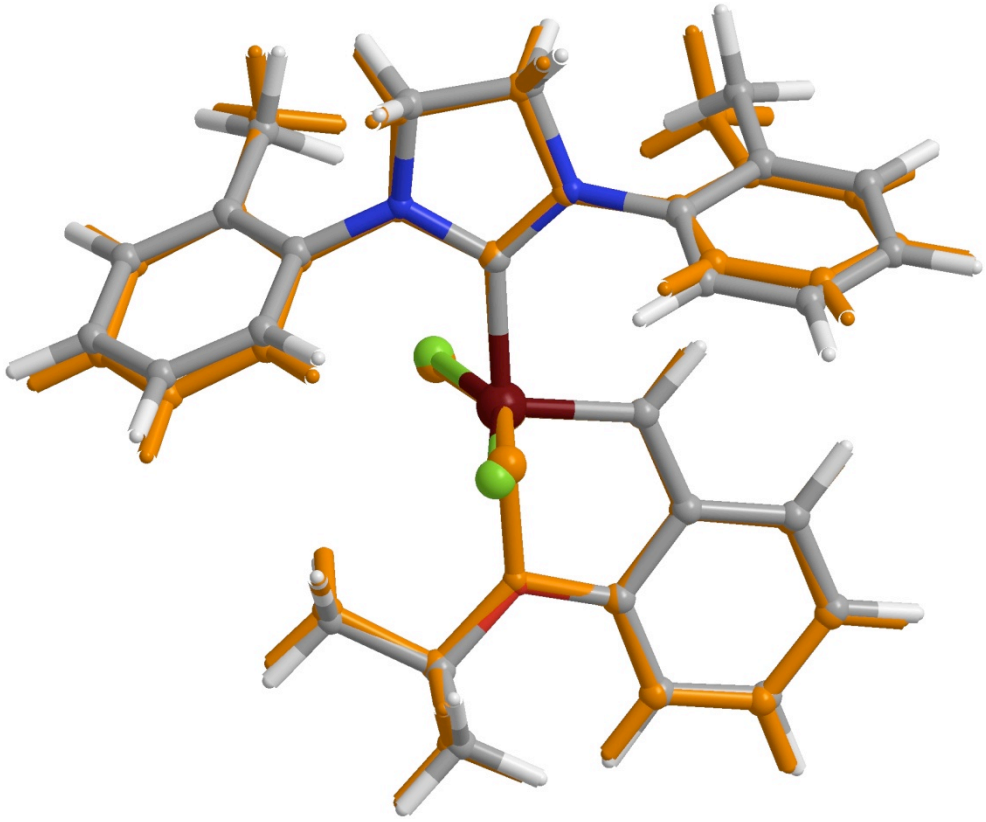
Geometry/Energy	SP Gas Phase LACV3P**++(2f)	LACVP** CH_2CL_2	B3LYP/LACVP** gas phase Optimization Analytic Hessian		
	E_{SCF}	**Vsolv**	**Hvib**	**ZPE**	**Svib**
B3LYP/B3LYP					
3d	-2246.426644	-14.2813	19.373	321.483	127.25056
3b	-2246.426976	-14.3458	19.393	321.469	127.60973
3c	-2246.427469	-14.6046	19.341	321.625	127.32037
3a	-2246.427469	-14.3899	19.37	321.595	127.70626
B3LYP/M06					
3d	-2245.40703	-14.6177	19.373	321.483	127.25056
3b	-2245.407782	-14.6894	19.393	321.469	127.60973
3c	-2245.407088	-14.9578	19.341	321.625	127.32037
3a	-2245.407882	-14.745	19.37	321.595	127.70626
M06-L/M06					
3d	-2245.406645	-15.3701	19.373	321.483	127.25056
3b	-2245.407311	-15.0758	19.393	321.469	127.60973
3c	-2245.407679	-15.5123	19.341	321.625	127.32037
3a	-2245.408321	-15.4764	19.37	321.595	127.70626

	Geometry MO6-L/ LACVP+**	Geometry MO6-L/ LACVP+**	Geometry B3LYP/LACVP+**		
Complex	Single Point Energy Gas Phase MO6/LACV3P++**(2f)	MO6/LACVP+** CH_2Cl_2	Analytic Hessian		
	E_{SCF}	**Vsolv**	**Hvib**	**ZPE**	**Svib**
5a	-2129.677242	-23.2186	16.745	286.031	113.7118
5b	-2129.677569	-21.4698	17.305	286.142	113.7135
5c	-2129.675997	-21.8468	16.575	286.197	111.4614
5d	-2129.674211	-22.7799	16.648	286.02	112.1315
5e	-2129.671264	-20.8354	16.188	285.981	113.4256
5f	-2129.669191	-23.0595	16.084	285.981	112.4291
5g	-2129.668002	-21.1299	16.111	286.037	112.0403
5h	-2129.67639	-15.3855	16.384	285.842	115.4433
5i	-2129.675931	-15.5148	16.884	285.829	114.6841
5j	-2129.675945	-15.5397	16.763	286.01	113.2571
5k	-2129.663656	-22.4721	16.13	285.866	112.3851
5l	-2129.674172	-15.35	16.865	285.84	114.0773

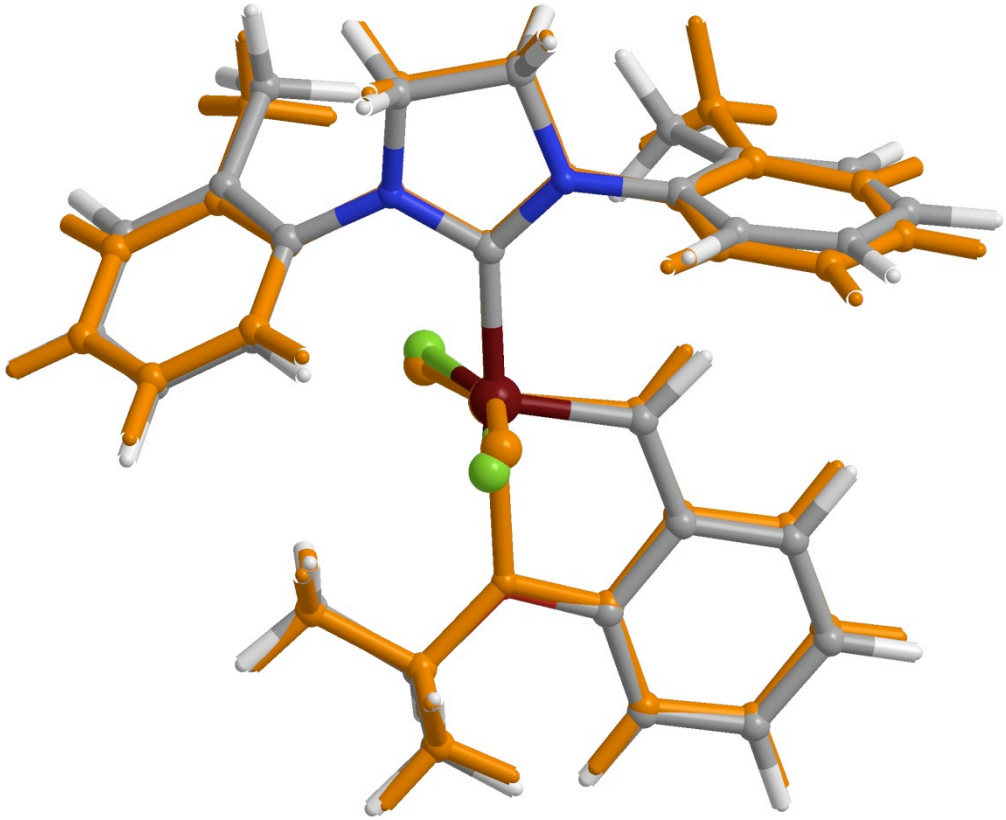
	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**		
Complex	Single Point Energy Gas Phase MO6/LACV3P**++(2f)	MO6/LACVP+** CH_2Cl_2	Gas Phase Optimization Analytic Hessian		
	E_{SCF}	**Vsolv**	**Hvib**	**ZPE**	**Svib**
5a	-2129.675324	-21.7887	16.745	286.031	113.7118
5b	-2129.676886	-21.0393	17.305	286.142	113.7135
5c	-2129.676278	-21.0802	16.575	286.197	111.4614
5d	-2129.674062	-21.3056	16.648	286.02	112.1315
5e	-2129.672999	-20.7455	16.188	285.981	113.4256
5f	-2129.674483	-21.9691	16.084	285.981	112.4291
5g	-2129.671134	-21.7221	16.111	286.037	112.0403
5h	-2129.675494	-15.0037	16.384	285.842	115.4433
5i	-2129.674838	-15.068	16.884	285.829	114.6841
5j	-2129.67511	-15.3562	16.763	286.01	113.2571
5k	-2129.671676	-21.7432	16.13	285.866	112.3851
5l	-2129.674077	-15.0605	16.865	285.84	114.0773

	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**	Geometry B3LYP/ LACVP+**		
Complex	Single Point Energy Gas Phase B3LYP/LACV3P**++(2f)	B3LYP/LACVP+** CH_2Cl_2	Gas Phase Optimization Analytic Hessian		
	E_{SCF}	**Vsolv**	**Hvib**	**ZPE**	**Svib**
5a	-2130.623446	-21.9926	16.745	286.031	113.7118
5b	-2130.625229	-21.1875	17.305	286.142	113.7135
5c	-2130.625273	-21.2182	16.575	286.197	111.4614
5d	-2130.622654	-21.4997	16.648	286.02	112.1315
5e	-2130.621468	-21.0416	16.188	285.981	113.4256
5f	-2130.622153	-22.2292	16.084	285.981	112.4291
5g	-2130.620668	-21.9096	16.111	286.037	112.0403
5h	-2130.628653	-14.8596	16.384	285.842	115.4433
5i	-2130.627521	-14.87	16.884	285.829	114.6841
5j	-2130.628004	-15.1605	16.763	286.01	113.2571
5k	-2130.619641	-21.9885	16.13	285.866	112.3851
5l	-2130.627643	-14.8966	16.865	285.84	114.0773

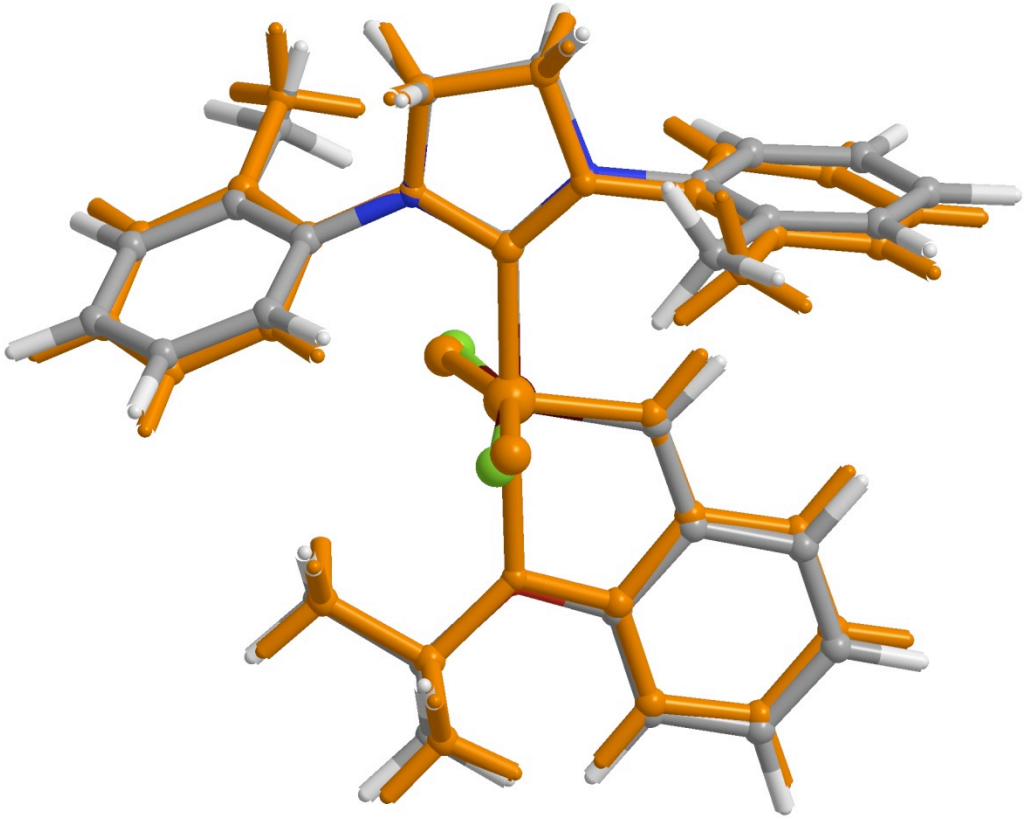
3a X-Ray in Orange, B3LYP minimized in color.



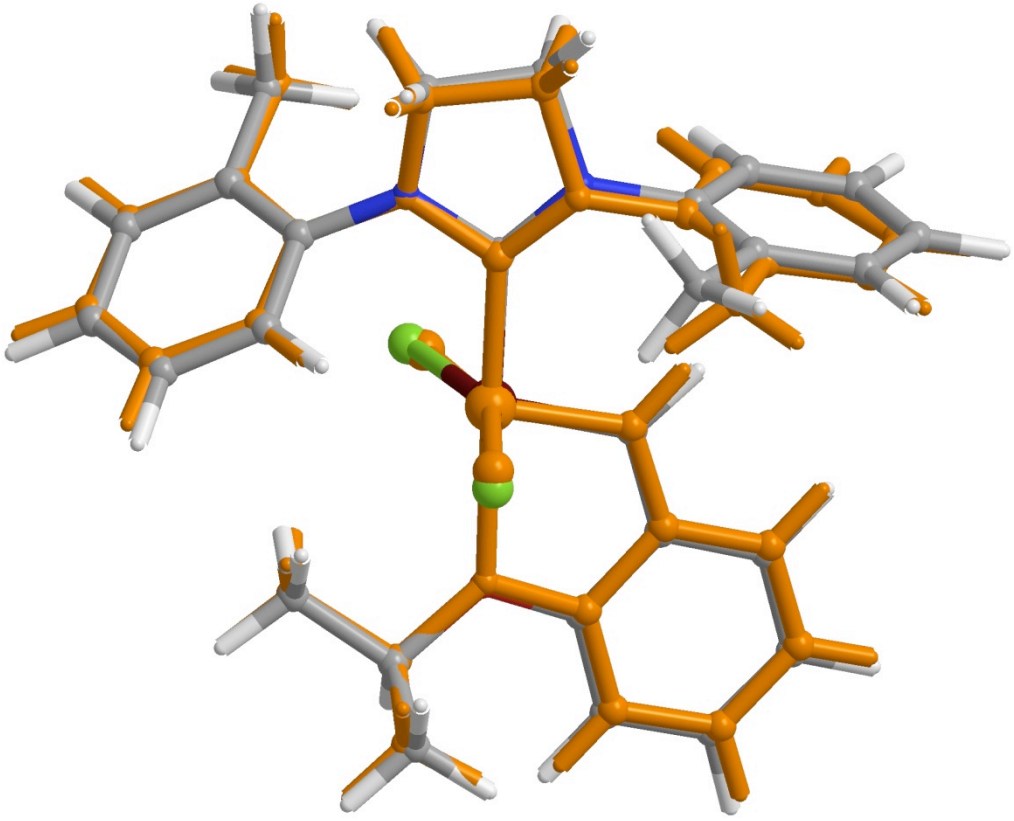
3a X-Ray in Orange, M06-L minimized in color.



3b X-Ray in Orange, B3LYP minimized in color.



3b X-Ray in Orange, M06-L minimized in color.



XYZ coordinates

a) B3LYP optimized geometries

3a

N1	0.3180701199	0.1904840695	-0.5470926453
C2	1.7922907050	0.1706389742	-0.5551975006
C3	2.0919360378	-0.4900344041	-1.9025352467
N4	0.7895516591	-1.0929907171	-2.2593440820
C5	-0.3934350378	1.0271296225	0.3746583835
C6	-1.7163180278	2.7630905413	2.1068424411
C7	-1.0939109238	2.1267060203	-0.1322441175
C8	-0.3379945197	0.7772647514	1.7610123226
C9	-1.0080469088	1.6691522726	2.6051420415
C10	-1.7658377413	2.9903116449	0.7334941884
H11	-0.9887675854	1.4856525004	3.6766132920
H12	-2.3136153639	3.8373816403	0.3310824151
C13	-0.2359445121	-0.5760932998	-1.5267195861
Ru14	-2.2134733840	-0.7377174266	-1.6842049046
Cl15	-2.4090555664	-1.7766981823	0.4764194849
Cl16	-2.2958670979	1.0475266978	-3.3163383342
C17	-2.3379257082	-2.2396418787	-2.7428927886
H18	-1.4815244461	-2.8278132572	-3.0749978520
C19	0.7192734697	-1.7935740012	-3.5075675902
C20	0.7091168105	-3.0994350650	-5.9630155537
C21	1.1711719427	-3.1266470033	-3.5690009416
C22	0.2730235390	-1.1238151835	-4.6498455925
C23	0.2611059872	-1.7811723463	-5.8789908765
C24	1.1565782166	-3.7599706921	-4.8182893443
H25	-0.0998308586	-1.2641430978	-6.7630832388
H26	1.4930289710	-4.7915766992	-4.8880782303
H27	2.3797338064	0.2362890882	-2.6734036833
H28	2.1900120169	1.1861103756	-0.4768085147
H29	2.1744680762	-0.4190871469	0.2853381924
H30	2.8731867020	-1.2510813931	-1.8402731889
C31	-3.6314613581	-2.7212127074	-3.1715950625
C32	-6.1633378124	-3.6031328896	-3.9783517474
C33	-3.7688996773	-3.8330714301	-4.0239353474
C34	-4.8045237790	-2.0571531212	-2.7298041037
C35	-6.0662553133	-2.4974288975	-3.1295221860
C36	-5.0236001263	-4.2746031249	-4.4280909786
H37	-6.9677188382	-2.0006710954	-2.7933391508
H38	-7.1484719659	-3.9418477667	-4.2872957039
O39	-4.5616277232	-0.9862926646	-1.9208100916
C40	-5.6552523147	-0.3097201532	-1.2190355015
H41	-6.4497967940	-0.1493517577	-1.9572522607
H42	-2.8687025134	-4.3388455396	-4.3634015512
H43	-5.1183975782	-5.1337238044	-5.0849683525
C44	-5.1170651136	1.0410391079	-0.7731126393
H45	-4.3353970195	0.9164373439	-0.0177317545
H46	-5.9324781713	1.6225273933	-0.3297654417
H47	-4.7052449760	1.5933750097	-1.6209902483
C48	-6.1441947730	-1.1735225813	-0.0598401153
H49	-5.3212384819	-1.3512614722	0.6373755242
H50	-6.5217123557	-2.1411075257	-0.4011079841
H51	-6.9555451140	-0.6579506508	0.4652689057
H52	-2.2312522360	3.4305066129	2.7925458233
H53	0.7059805317	-3.6178754085	-6.9180186845
H54	-0.1009062082	-0.1094578525	-4.5529145147
C55	1.6259067562	-3.8681290316	-2.3333308687
H56	2.6212666888	-3.5445681046	-2.0022655183
H57	1.6846524713	-4.9424411771	-2.5281067625
H58	0.9398440198	-3.7068486612	-1.4961745616
H59	-1.1175695021	2.2885271453	-1.2049747968
C60	0.3744077700	-0.4221080046	2.3362356576
H61	1.4594010967	-0.2671934157	2.3966042070
H62	0.1806235951	-1.3116702598	1.7311539885
H63	0.0207800939	-0.6239831085	3.3508107590

3b

N1	0.2990338462	0.3559206087	-0.6756831056
C2	1.7049788465	0.7129320450	-0.9400510149
C3	2.1041763864	-0.3505597370	-1.9600898547
N4	0.7892397781	-0.7823388313	-2.4785651558
C5	-0.4185062405	1.0829754677	0.3355048737
C6	-1.6969704634	2.5935528972	2.2919465561
C7	-1.1871656120	2.1916716191	-0.0290029518
C8	-0.2617893202	0.7150404201	1.6882476370
C9	-0.9164771759	1.4924779516	2.6488462170
C10	-1.8362232333	2.9441986131	0.9512351012
H11	-0.8201940952	1.2187270984	3.6964808895
H12	-2.4392433133	3.7999550404	0.6623451942
C13	-0.2370341988	-0.4196285307	-1.6622764021
Ru14	-2.2075929064	-0.7173977250	-1.7278265411
Cl15	-2.1762253203	-2.0474972082	0.2750453956
Cl16	-2.5339130118	1.2458359582	-3.1078888297
C17	-2.3611138533	-2.0238483226	-3.0182518429
H18	-1.5173258759	-2.4879438505	-3.5261146999
C19	0.7878931482	-1.7562360519	-3.5289134116
C20	0.9320126643	-3.6687747350	-5.5415285992
C21	0.9850989760	-3.1010019125	-3.2024538659
C22	0.6760770295	-1.3364962000	-4.8675126647
C23	0.7469295590	-2.3230629740	-5.8601306212
C24	1.0535549416	-4.0633256827	-4.2087349018
H25	0.6539675453	-2.0252062718	-6.9014632091
H26	1.1962585510	-5.1090796273	-3.9529935322
H27	2.7310031887	0.0348151803	-2.7682578250
H28	1.7572641011	1.7290948539	-1.3536222576
H29	2.3005993704	0.6805307666	-0.0251288207
H30	2.6209925608	-1.2014783743	-1.4966638222
C31	-3.6668956620	-2.4920303211	-3.4248051837
C32	-6.2214537551	-3.3425854078	-4.1905884823
C33	-3.8315875956	-3.4411535613	-4.4513019315
C34	-4.8233467235	-1.9772860441	-2.7859074333
C35	-6.0966092667	-2.4022142158	-3.1644140313
C36	-5.0982580248	-3.8656641010	-4.8363667023
H37	-6.9854383782	-2.0189261705	-2.6791789843
H38	-7.2154316865	-3.6693024196	-4.4836171527
O39	-4.5509609476	-1.0557710867	-1.8186693136
C40	-5.6080989597	-0.5482977896	-0.9414544476
H41	-6.4601390238	-0.3036202690	-1.5864232623
H42	-2.9434109630	-3.8334171853	-4.9400509701
H43	-5.2147973415	-4.5972354750	-5.6299092362
C44	-5.0776284286	0.7329919787	-0.3169483150
H45	-4.2352220440	0.5198288296	0.3476930294
H46	-5.8724845103	1.1986623265	0.2753840814
H47	-4.7513197696	1.4338097506	-1.0888885411
C48	-5.9810821723	-1.6104569226	0.0887019252
H49	-5.1021236330	-1.8648970367	0.6867397550
H50	-6.3538789044	-2.5239916572	-0.3823165413
H51	-6.7651889924	-1.2234946279	0.7483457150
H52	-2.1953989288	3.1733311711	3.0641488051
H53	0.9846472365	-4.4082492969	-6.3359974953
H54	-1.2875126798	2.4425869733	-1.0794336180
C55	0.5496635690	-0.4889384526	2.0962037060
H56	1.6142688627	-0.3698745721	1.8597557950
H57	0.1850725254	-1.3818177389	1.5801022749
H58	0.4711704447	-0.6576366909	3.1735344326
H59	1.0587284004	-3.3843220693	-2.1563302702
C60	0.4675566404	0.1145358035	-5.2228469863
H61	1.2901556395	0.7396788458	-4.8553665802
H62	-0.4539445452	0.5055879999	-4.7779343978
H63	0.4111804073	0.2408013916	-6.3073060611

3c

N1	0.2637518788	0.7958344589	-1.1148951479
C2	1.7363437320	0.8287627508	-1.1874865762
C3	2.0040712592	0.0100253931	-2.4511747564
N4	0.7339782540	-0.7299921445	-2.6178839831
C5	-0.3869197799	1.4687955230	-0.0252237708
C6	-1.5409537966	2.7488607290	2.1601976733
C7	-0.5858455986	2.8629001575	-0.0832029981
C8	-0.7446047809	0.7329350993	1.1083693760
C9	-1.3328724817	1.3724005512	2.2007184660

C10	-1.1666839272	3.4782761445	1.0304741083
C11	-0.2350533454	3.6667703926	-1.3100168933
H12	-1.6165581465	0.7941468208	3.0752648798
H13	-1.3418428116	4.5507706990	1.0020578811
H14	-0.5658796123	4.7027373961	-1.1971123543
H15	-0.7270152617	3.2412395039	-2.1895722242
C16	-0.2732033354	-0.2112616094	-1.8624552776
Ru17	-2.1980460573	-0.6812610975	-1.7135543608
Cl18	-1.7370887847	-2.4368678090	-0.1105172551
Cl19	-2.9012019771	1.4898669608	-2.4622527781
C20	-2.4288443639	-1.5805857136	-3.3043903360
H21	-1.6416094625	-1.7202369490	-4.0459978606
H22	0.8451692689	3.6872100336	-1.5005342152
C23	0.7240155992	-1.9191504699	-3.4153820668
C24	0.8344054274	-4.2708266395	-4.9028072793
C25	0.6153907113	-3.1580934660	-2.7754050019
C26	0.8844436330	-1.8329120373	-4.8129326303
C27	0.9413612881	-3.0323556939	-5.5351966297
C28	0.6616928475	-4.3354693494	-3.5197537421
H29	1.0579267953	-2.9874310768	-6.6155602878
H30	0.5660857181	-5.2942274240	-3.0194709868
C31	0.9546865434	-0.5047995444	-5.5312925320
H32	1.9694867221	-0.0872524800	-5.5222696265
H33	0.2897759278	0.2333923474	-5.0727414184
H34	0.6651706704	-0.6180728077	-6.5798589025
H35	2.1904443924	0.6510534736	-3.3209400553
H36	2.1069851573	1.8540427832	-1.2571706985
H37	2.1624349918	0.3666752049	-0.2867901039
H38	2.8392564493	-0.6865170161	-2.3462353648
C39	-3.7259180810	-2.1042455591	-3.6658192750
C40	-6.2670465799	-3.0775259329	-4.3227806064
C41	-3.9523787106	-2.7557221980	-4.8931018927
C42	-4.8138567937	-1.9512929797	-2.7685218029
C43	-6.0797127129	-2.4388188209	-3.0941837433
C44	-5.2123235056	-3.2403506589	-5.2245658727
H45	-6.9159617914	-2.3314532753	-2.4149333978
H46	-7.2554073025	-3.4535165896	-4.5724976057
O47	-4.4921563874	-1.2899346492	-1.6205401719
C48	-5.4612102793	-1.1532827187	-0.5318132796
H49	-6.4166155141	-0.8785675349	-0.9937600248
H50	-3.1169320222	-2.8718946053	-5.5786187934
H51	-5.3765014568	-3.7405397651	-6.1739761005
C52	-4.9842192556	0.0011725070	0.3362075970
H53	-4.0382518481	-0.2478026536	0.8261728424
H54	-5.7311249768	0.1985122320	1.1125860548
H55	-4.8437856786	0.9045110254	-0.2618519263
C56	-5.5729698040	-2.4730810553	0.2258406492
H57	-4.5979457791	-2.7407569016	0.6415682366
H58	-5.9064377722	-3.2883222047	-0.4220700978
H59	-6.2955170795	-2.3698864649	1.0424767552
H60	-0.5768867588	-0.3390719522	1.1186947372
H61	-1.9949924301	3.2590750157	3.0054499213
H62	0.8783036536	-5.1823782701	-5.4925978157
H63	0.4584108615	-3.1809748797	-1.7020482294

3d

N1	0.2927545260	0.5915238339	-0.9360385202
C2	1.7647105823	0.5364556847	-0.8633116581
C3	2.1021441823	-0.2906415925	-2.1016220978
N4	0.8198395478	-0.9759767707	-2.3677378863
C5	-0.4137305682	1.3761547600	0.0396527501
C6	-1.6447505560	2.9019623563	2.0147981976
C7	-0.5633578354	2.7629896483	-0.1689073898
C8	-0.8519246315	0.7699652663	1.2203602487
C9	-1.4781630509	1.5323185660	2.2071038353
C10	-1.1879140870	3.5035593744	0.8408580918
C11	-0.0995628430	3.4316116835	-1.4389856980
H12	-1.8246579260	1.0546548470	3.1188749253
H13	-1.3232211515	4.5726650407	0.6971965012
H14	-0.3146363008	4.5033399581	-1.4091375268
H15	-0.6149049402	2.9973595226	-2.3013027790
C16	-0.2285962825	-0.3865496782	-1.7325963852
Ru17	-2.1908463099	-0.7424834115	-1.7095804205
Cl18	-1.9685722822	-2.3084541732	0.1286004291
Cl19	-2.6833520159	1.3175681684	-2.8466944638
C20	-2.3944589984	-1.9169586336	-3.1150382652
H21	-1.5795806273	-2.2685858425	-3.7455968745
H22	0.9793111317	3.3153872773	-1.5990431136
C23	0.7927897720	-1.9214943925	-3.4430596004
C24	0.8785118827	-3.7063893411	-5.5722609189
C25	0.9627713254	-3.2913345484	-3.1682380273
C26	0.6834994004	-1.4502406572	-4.7542268695
C27	0.7214776096	-2.3430000565	-5.8241381618
C28	0.9974413358	-4.1679656901	-4.2607760483
H29	0.6256404631	-1.9767111759	-6.8419397123
H30	1.1189847446	-5.2320755222	-4.0745638058
H31	2.3762499733	0.3351629543	-2.9615719920
H32	2.1997572178	1.5386198354	-0.8796975396
H33	2.0714586104	0.0398238087	0.0671329734
H34	2.9015750856	-1.0171856448	-1.9350217838
C35	-3.7064553734	-2.4175171762	-3.4570200905
C36	-6.2713677869	-3.3475842824	-4.0831633012
C37	-3.9111893912	-3.2861719828	-4.5457977107
C38	-4.8279234587	-2.0250839781	-2.6829314993
C39	-6.1060995045	-2.4890638923	-2.9929595921
C40	-5.1830339066	-3.7508481288	-4.8612957423
H41	-6.9682742510	-2.1990216471	-2.4057601990
H42	-7.2692151409	-3.7059158472	-4.3212346454
O43	-4.5207857974	-1.1740690534	-1.6632222015
C44	-5.5342635305	-0.7715998456	-0.6856348295
H45	-6.4384126384	-0.5260103372	-1.2547853459
H46	-3.0495251710	-3.5860245411	-5.1366011136
H47	-5.3306209177	-4.4210655295	-5.7025653386
C48	-5.0182596544	0.4911258765	-0.0126555550
H49	-4.1248788529	0.2775838661	0.5819323331
H50	-5.7910920148	0.8800912199	0.6589856217
H51	-4.7726194890	1.2543507260	-0.7545261755
C52	-5.7912187044	-1.9134003256	0.2938013335
H53	-4.8639220636	-2.1657268723	0.8149022127
H54	-6.1563589718	-2.8117971555	-0.2111128976
H55	-6.5438762843	-1.6057798854	1.0277568758
H56	-0.7205938033	-0.2992168435	1.3445339338
H57	-2.1277046699	3.5069339264	2.7777344237
H58	0.9111365510	-4.4130742323	-6.3972014032
H59	0.5436767794	-0.3860497774	-4.9216460135
C60	1.0805509278	-3.8017884250	-1.7533233812
H61	1.9458341034	-3.3655437714	-1.2398732304
H62	1.2012400524	-4.8883456736	-1.7452573770
H63	0.1947916256	-3.5456061124	-1.1617714477

5a

Ru1	0.0342766102	-0.0055620779	0.0383319671
Cl2	0.0731184928	2.4347608302	0.0605164592
Cl3	-2.4205673215	0.2192085497	0.0393459201
N4	-0.3244873369	-2.0086016652	-2.1111598391
N5	-0.8622257489	-3.0022741479	-0.2345831360
C6	-0.3892937798	-1.8559012890	-0.7638967615
C7	-1.0240022064	-3.2257809938	-2.5745567501
H8	-0.4320059020	-3.7614966987	-3.3202722305
H9	-1.9842445059	-2.9452770148	-3.0238144299
C10	-1.1937834789	-4.0127980832	-1.2679878342
H11	-2.2142240818	-4.3756381664	-1.1189063568
H12	-0.5081100996	-4.8648407545	-1.1995299468
C13	0.0493563211	-0.9752970160	-3.0366159273
C14	1.1616083758	-1.1736649305	-3.8844434847
C15	1.4803492802	-0.1492361555	-4.7855345243
H16	2.3372627309	-0.2766507908	-5.4426073056
C17	0.7354127946	1.0321941133	-4.8441351984
C18	-0.3568625271	1.2109003725	-3.9962526183
H19	-0.9339121688	2.1295570292	-4.0200707649
C20	-0.7103326298	0.2000967000	-3.0994223230
C21	1.9965978372	-2.4334332648	-3.8417208234
H22	2.0923826447	-2.8218245051	-2.8232556757
H23	3.0014010492	-2.2428770069	-4.2294765516

H24	1.5607633871	-3.2317717993	-4.4571132518
C25	-1.0904429271	-3.3265139948	1.1458847681
C26	-0.2244626338	-4.2210341357	1.8062356192
C27	-0.5408998432	-4.5793708869	3.1250265360
H28	0.1203090216	-5.2594550591	3.6565092710
C29	-1.6723867774	-4.0738897069	3.7666831188
C30	-2.5154935421	-3.1841735525	3.0962546667
H31	-3.3939520554	-2.7783712206	3.5891486842
C32	-2.2270550402	-2.8144584251	1.7823326286
C33	1.0081714434	-4.7957213472	1.1471010870
H34	0.7891332287	-5.7488429407	0.6479760638
H35	1.7849877549	-4.9926540843	1.8914140064
H36	1.4237179134	-4.1158478217	0.3991156647
C37	0.0665390441	-0.3830920469	1.8480641191
H38	-0.8245276316	-0.1570726817	2.4398349739
C39	1.2591538331	-0.8468729740	2.5256590310
C40	1.3700639364	-1.0136173543	3.9196994319
H41	0.5260229345	-0.7697745111	4.5588394748
C42	2.5584800348	-1.4980298116	4.4626830526
H43	2.6522092582	-1.6299779301	5.5366306392
C44	3.6339935669	-1.8190116010	3.6232810415
H45	4.5580082843	-2.1964616458	4.0525978771
C46	3.5350024162	-1.6484343552	2.2365365099
H47	4.3802920999	-1.8860204972	1.5957904201
C48	2.3536920037	-1.1504109042	1.6852898550
C49	2.1458761137	-0.8972299126	0.2325319860
H50	2.2609156932	-1.7521156794	-0.4308474515
C51	2.2104197565	0.3849225015	-0.3051026838
H52	2.4533938208	1.2401814211	0.3141564023
H53	2.3297604790	0.5275318420	-1.3759565967
H54	-1.5657578253	0.3207570844	-2.4403417425
H55	-2.8512228061	-2.1073567473	1.2453580149
H56	1.0166857355	1.8123045618	-5.5456581851
H57	-1.8906613748	-4.3700714958	4.7890288197

5b

C1	-0.0089609191	0.0000413645	-0.1820153152
C2	0.0139068537	2.8120670865	-0.1342026481
C3	-1.2052635618	0.7235465301	-0.2507420851
H4	4.6252020406	3.0558761924	4.8697452420
Ru5	4.0888568598	1.6950403255	0.0393584695
Cl6	4.5451371262	0.8485469814	-2.1763037617
Cl7	5.4457111811	3.6669802937	-0.5178230035
C8	3.2853933468	-0.1196870431	1.1280576312
N9	4.3102865457	3.2202572078	2.7748644133
N10	5.7788256960	1.6207913719	2.5065594534
C11	3.4887022841	5.3672700574	1.9753698672
C12	1.9726610530	3.8809158787	3.1932746238
C13	2.5361724461	2.7043869044	-0.0197449763
C14	3.2295351634	4.1511744146	2.6180811517
C15	4.6986215074	2.2273213209	1.9499252208
C16	0.9859501914	4.8737008951	3.0931277207
C17	1.2355328283	6.0878081918	2.4507555912
C18	6.5608725552	0.5759592898	1.9051876034
C19	8.1317264243	-1.4181259293	0.7544838064
C20	6.6897695967	-0.6611342769	2.5746774010
C21	7.4881720619	-1.6435278905	1.9746089642
H22	2.8818867855	0.1767431621	2.0910628724
H23	4.1051404133	-0.8324159974	1.1526206535
H24	2.6076268053	3.7864610479	-0.1494442494
H25	0.0072345996	4.6860275475	3.5275327975
H26	7.5947891613	-2.6064974757	2.4682078207
C27	7.2110256259	0.8126882540	0.6881315888
C28	1.2232492591	2.0924894719	-0.0587422555
C29	7.9880642748	-0.1918140474	0.1068631115
C30	1.6592956129	2.5622285824	3.8594611885
C31	5.9972608165	-0.9450618957	3.8881227162
C32	6.3304536270	2.3921037710	3.6418572402
C33	2.4894572725	6.3362310556	1.8859926349
C34	5.1787691806	3.3486321132	3.9685962854
C35	-1.1950314175	2.1252379798	-0.2234400899
C36	2.5334656414	0.0124670633	-0.0321524984
H37	-0.0246672917	-1.0859152090	-0.2168083276
H38	0.0362592018	3.8982698183	-0.1317206807
H39	-2.1494679146	0.1926487454	-0.3349244183
H40	-2.1296807160	2.6748071384	-0.2883717849
H41	8.4695629535	-0.0088172038	-0.8482710629
H42	6.5918919852	1.7362584169	4.4749260593
H43	2.6892082519	7.2741310137	1.3767026546
H44	5.5048248132	4.3852129719	4.0862625036
H45	0.7806265512	2.6536715382	4.5038661394
H46	2.4901078777	2.1943566269	4.4689188222
H47	1.4394863394	1.7931158281	3.1095667843
H48	6.5873370842	-0.5903151448	4.7434982371
H49	5.8539622634	-2.0209959002	4.0235566442
H50	5.0177962383	-0.4607580737	3.9418930398
H51	7.2337742574	2.9210103750	3.3144190372
C52	1.2063536394	0.6789893897	-0.0725388039
H53	2.8057549874	-0.5795826559	-0.9014547265
H54	0.4521055273	6.8384550571	2.3929325919
H55	8.7358250057	-2.2041889722	0.3105745861
H56	4.4609638400	5.5187156401	1.5178419180
H57	7.0975761996	1.7764419088	0.2002690189

5c

C1	-0.0633323032	0.1544674600	-0.1581419339
C2	0.0850100967	2.9579338111	-0.3199209650
C3	-1.2202529250	0.9193567533	-0.3450015817
H4	4.7374228944	3.1511108612	4.7463622108
Ru5	4.0881366159	1.6742594758	0.0504867738
Cl6	4.4399902152	0.6276428915	-2.1019901068
Cl7	5.5224663407	3.5113115209	-0.7252205142
C8	3.1667313632	0.0607579157	1.3352312468
N9	4.4578515020	3.4030131970	2.6621319349
N10	5.8500629614	1.7251795131	2.4586605658
C11	3.4026394348	5.5795133185	2.2079502839
C12	2.0647740500	3.7056713782	3.0356639858
C13	2.5910692732	2.7559289827	-0.0786746147
C14	3.2870212803	4.2297673486	2.6006077718
C15	4.7739084289	2.3345726619	1.8965986631
C16	0.9233338860	4.5066274815	3.0676857669
C17	1.0148742634	5.8422917194	2.6718290702
C18	6.5742827541	0.6116842323	1.9078173751
C19	8.0317680256	-1.5210732108	0.8603906929
C20	6.6726226435	-0.5810110163	2.6588564774
C21	7.4134967384	-1.6349946825	2.1087041494
H22	2.7430484780	0.5039705271	2.2315247578
H23	3.9428807427	-0.6833489314	1.4917615820
H24	2.7118492096	3.8292364206	-0.2463792034
H25	-0.0239827386	4.0896030077	3.3953930991
H26	7.4954792657	-2.5651667333	2.6657487582
C27	7.2008664423	0.7370353114	0.6622785199
C28	1.2554341233	2.1971735043	-0.1292770829
C29	7.9206542611	-0.3367919720	0.1334912988
C30	6.0115203672	-0.7437385107	4.0086263989
C31	6.4611749377	2.5551316435	3.5191547917
C32	2.2397790064	6.3638455028	2.2495109592
C33	5.3087262040	3.4931143405	3.8728224410
C34	-1.1477435325	2.3173678925	-0.4222051567
C35	2.4624789397	0.0695066344	0.1365850844
H36	-0.1266421076	-0.9292787072	-0.1103899336
H37	0.1560917134	4.0392539567	-0.3979847603
H38	-2.1821666799	0.4231216750	-0.4392213648
H39	-2.0520219345	2.8985446714	-0.5779368909
C40	4.7141932964	6.1683663134	1.7490895710
H41	8.3826764121	-0.2395934460	-0.8435628512
H42	6.7949839079	1.9441219220	4.3597574106
H43	2.3014982504	7.4039710291	1.9402407361
H44	5.6294547708	4.5221982719	4.0473930584
H45	5.4157158110	6.2912975800	2.5848351251
H46	4.5563532701	7.1581036005	1.3118453866
H47	6.6361167279	-0.3420283924	4.8175173588
H48	5.8441185913	-1.8016547198	4.2303541070
H49	5.0474584185	-0.2284651644	4.0533451742

H50	7.3244622505	3.0916360359	3.1051068058
C51	1.1747238448	0.7886084608	-0.0364400898
H52	5.1920139597	5.5275415088	1.0011748057
H53	2.7251021826	-0.6521878506	-0.6313885716
H54	0.1349535119	6.4792669023	2.6918003945
H55	8.5908909003	-2.3606025147	0.4572835356
H56	2.0145835747	2.6650041695	3.3416478452
H57	7.1122056386	1.6680409028	0.1105134638

5d

Ru1	0.0268242017	0.0026622846	-0.0026516268
Cl2	-0.0288942420	2.4426084691	-0.0153747311
Cl3	-2.4198948690	0.1334213735	-0.1655434274
N4	-0.0495782224	-2.0086750787	-2.1746282927
N5	-0.7639638354	-3.0225130766	-0.3683394180
C6	-0.2519591474	-1.8648171714	-0.8373173001
C7	-0.6828772485	-3.2380614980	-2.6993560898
H8	-0.0500188986	-3.7252604997	-3.4439649780
H9	-1.6442515683	-2.9826025361	-3.1629250912
C10	-0.8525949920	-4.0614110593	-1.4222138312
H11	-1.8103925950	-4.5837914813	-1.3716011266
H12	-0.0468510468	-4.7942437139	-1.2817689797
C13	0.3320149083	-0.9465585186	-3.0643909107
C14	1.5048304113	-1.0844150937	-3.8391859592
C15	1.8353312515	-0.0354711931	-4.7068795594
H16	2.7382565180	-0.1161197625	-5.3072661332
C17	1.0429502129	1.1125147173	-4.8028126227
C18	-0.1104275626	1.2301963745	-4.0288586770
H19	-0.7257516878	2.1224577794	-4.0811364443
C20	-0.4762416167	0.1925248907	-3.1680937408
C21	2.3896196287	-2.3071960083	-3.7528936184
H22	2.4464111861	-2.6942759398	-2.7310275545
H23	3.4043632803	-2.0730784442	-4.0868551399
H24	2.0211352723	-3.1212357418	-4.3913868311
C25	-0.9375761729	-3.4311218290	0.9975710049
C26	0.1926559371	-3.7851727919	1.7427771224
C27	0.0586516383	-4.2713260299	3.0431897923
H28	0.9408257779	-4.5324892543	3.6193963665
C29	-1.2179343924	-4.4096138687	3.5916172507
C30	-2.3431574639	-4.0684167450	2.8383348428
H31	-3.3332983073	-4.1794235991	3.2727897517
C32	-2.2359806066	-3.5819775195	1.5262314627
C33	-3.4705174541	-3.2446393196	0.7270844833
H34	-3.3753978310	-2.2629324337	0.2536803835
H35	-4.3529220417	-3.2349164608	1.3729121579
H36	-3.6535655788	-3.9878048650	-0.0605371646
C37	-0.0848457915	-0.3208414289	1.8143362931
H38	-1.0516903451	-0.1773592352	2.3046196880
C39	1.0792088665	-0.6111568736	2.6237371694
C40	1.0782107140	-0.6632629214	4.0307357245
H41	0.1601601889	-0.4608245901	4.5754942147
C42	2.2542349686	-0.9791396934	4.7083957830
H43	2.2629658986	-1.0192377109	5.7937038887
C44	3.4272434483	-1.2485972138	3.9902968023
H45	4.3405050040	-1.4963151423	4.5241503276
C46	3.4378796009	-1.1932861049	2.5904395386
H47	4.3558026792	-1.3916229568	2.0432529519
C48	2.2687960194	-0.8622057577	1.9045222830
C49	2.1636638672	-0.7547849952	0.4218865060
H50	2.3499203974	-1.6661046542	-0.1441127851
C51	2.2158636604	0.4684286871	-0.2351367426
H52	2.3736412449	1.3905512673	0.3110154022
H53	2.4031538048	0.5125791986	-1.3047987580
H54	1.3340253270	1.9138338077	-5.4758755367
H55	-1.3794670117	0.2672204139	-2.5686112090
H56	-1.3398948111	-4.7842382220	4.6040856306
H57	1.1763290766	-3.6688116152	1.2985022904

5e

C1	-0.0541793802	-0.0369682879	0.0410201329
C2	-0.0325961533	2.7756999306	0.0649614581
C3	-1.2531489926	0.6846193811	0.0706307979
H4	4.8883315051	3.4900558654	4.7497022541
Ru5	4.0574909514	1.6773396335	-0.0537227769
Cl6	4.4955597947	0.7447171080	-2.2290264509
Cl7	5.2741737379	3.6811388207	-0.7509670452
C8	3.3365935943	-0.1798674988	1.0450341402
N9	4.3317885521	3.1337024472	2.7242081095
N10	5.9702443639	1.7556629622	2.2689013218
C11	3.4034896071	5.2393890211	1.9037182297
C12	2.0420610292	3.7845223276	3.3249469827
C13	2.4913432481	2.6715452812	-0.0175247483
C14	3.2282853404	4.0460168523	2.6130824413
C15	4.7802943492	2.2299065985	1.8205876409
C16	1.0327511841	4.7575190521	3.2857129587
C17	1.1967688264	5.9486073705	2.5753215064
C18	6.7267444612	0.6432197656	1.7537320115
C19	8.2218641454	-1.5574339809	0.9194975570
C20	6.4057427868	-0.6440902963	2.2065353497
C21	7.1443877637	-1.7493734989	1.7879474751
H22	3.0212860076	0.0879007105	2.0491483882
H23	4.1538540435	-0.8888215501	0.9675851673
H24	2.5458321820	3.7495953463	-0.1775178983
H25	0.1058972264	4.5748313563	3.8232876683
H26	6.8814115377	-2.7447068175	2.1333867523
C27	7.8451492869	0.8613985870	0.9238240838
C28	1.1798349163	2.0581777434	0.0452232123
C29	8.5644584610	-0.2704607646	0.5059323221
C30	1.8419510533	2.4980956270	4.0898198021
C31	6.3368289491	2.2910972368	3.5978437127
C32	2.3834162554	6.1908437370	1.8787509841
C33	5.3475150837	3.4446979914	3.7584663918
C34	-1.2432222258	2.0863528178	0.0848359130
C35	2.4904772812	-0.0138295344	-0.0396294952
H36	-0.0701390585	-1.1231805434	0.0146407734
H37	-0.0126041113	3.8616434847	0.0590805641
H38	-2.2000169665	0.1518314609	0.0726508537
H39	-2.1810987891	2.6341104825	0.0964281181
C40	8.2863885155	2.2419778633	0.5107132161
H41	9.4150645385	-0.1288555474	-0.1549490708
H42	6.2056986763	1.5108002868	4.3591601249
H43	2.5161509828	7.1104698601	1.3169452082
H44	5.8008254558	4.4191217407	3.5394958214
H45	0.9320968200	2.5449731425	4.6942082978
H46	2.6819389293	2.2825423656	4.7591677649
H47	1.7462885098	1.6458932922	3.4074558187
H48	7.5111902616	2.7571898406	-0.0645214206
H49	9.1932662113	2.1855492578	-0.0967259194
H50	8.5087072165	2.8662760158	1.3850080176
H51	7.3816279741	2.6124856948	3.6087633255
C52	1.1634514144	0.6459877295	0.0406915314
H53	2.6999862398	-0.5716188067	-0.9484309126
H54	0.3988396625	6.6859662564	2.5674885175
H55	8.8021946108	-2.4079366739	0.5733785284
H56	4.3215240101	5.3872889245	1.3432759007
H57	5.5705792085	-0.7701130771	2.8892837754

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Ru1	-0.0140207355	0.0717919189	0.0221151166
Cl2	-0.2381226728	2.4975098946	0.0396521722
Cl3	-2.4672120180	0.0483425350	-0.0550335553
N4	-0.2257763148	-1.8824420483	-2.1966766101
N5	-0.4192403347	-3.0360175836	-0.3446040017
C6	-0.2060585244	-1.7951737467	-0.8451205868
C7	-0.3668842929	-3.2716229831	-2.6793269507
H8	0.5998354464	-3.6323892638	-3.0557423765
H9	-1.0986592790	-3.3318590644	-3.4886651190
C10	-0.8132816865	-3.9941179446	-1.4080136193
H11	-1.8999175643	-4.1411287367	-1.3709505587
H12	-0.3235824054	-4.9597952386	-1.2657642280
C13	0.1259540648	-0.8352921517	-3.1177448773
C14	1.4818920663	-0.5664405218	-3.3468632159
C15	1.8641965512	0.4057634264	-4.2705284902
H16	2.9160543598	0.6173367870	-4.4374004531

C17	0.8780535482	1.0990138525	-4.9760136692
C18	-0.4703845383	0.8081974055	-4.7644883378
H19	-1.2291833073	1.3507273230	-5.3217186116
C20	-0.8824855231	-0.1675295892	-3.8438118626
C21	-2.3459238845	-0.4741384207	-3.6483050010
H22	-2.5750360254	-1.5200055518	-3.8883528103
H23	-2.9578870626	0.1555115934	-4.2993929331
H24	-2.6481173785	-0.3002082848	-2.6099512579
C25	-0.6773057293	-3.4191992600	1.0156878217
C26	0.2125564791	-4.3046497904	1.6566788601
C27	-0.1193517783	-4.7389562477	2.9479214939
H28	0.5583194211	-5.4138991532	3.4647827777
C29	-1.2902218704	-4.3165568961	3.5807046537
C30	-2.1581216611	-3.4381205399	2.9281582886
H31	-3.0693692651	-3.1001509125	3.4129191246
C32	-1.8549343828	-2.9934841437	1.6404395995
C33	1.4816069080	-4.7894338458	0.9947714078
H34	1.2915670767	-5.6411335632	0.3277104134
H35	2.2036155971	-5.1230796989	1.7451815890
H36	1.9500571093	-4.0029438496	0.3970035727
C37	-0.0164230461	-0.3564213386	1.8209714736
H38	-0.9441622847	-0.2188885465	2.3824696023
C39	1.1798966256	-0.7531684153	2.5344070717
C40	1.2415019246	-0.9824411016	3.9222480454
H41	0.3542162726	-0.8339037125	4.5313856029
C42	2.4364841734	-1.4122099409	4.4965205270
H43	2.4915368967	-1.5955660991	5.5655732913
C44	3.5677016802	-1.6147542188	3.6942472907
H45	4.4958733181	-1.9522446089	4.1472900653
C46	3.5182921378	-1.3773779167	2.3148159227
H47	4.4059920511	-1.5211044113	1.7040820988
C48	2.3294061091	-0.9343838976	1.7339896122
C49	2.1701515816	-0.6047265052	0.2914464986
H50	2.4220879092	-1.3893864318	-0.4191731118
C51	2.1218462694	0.7171406453	-0.1417045768
H52	2.2309100363	1.5357034960	0.5599689553
H53	2.2865874099	0.9685769320	-1.1849688158
H54	1.1578216417	1.8642280693	-5.6943131212
H55	-1.5204836155	-4.6704921380	4.5818029426
H56	-2.5049356985	-2.2974504894	1.1181733719
H57	2.2320701469	-1.1279696218	-2.7972493331

5g

C1	-0.2473588965	0.4053299843	0.2416929970
C2	0.1320509405	3.1561691210	-0.2038957842
C3	-1.3441892441	1.2560825667	0.0629744933
H4	4.8533586184	3.1936237408	4.7157973139
Ru5	4.0396238095	1.5585989868	0.0595343157
Cl6	4.2820606140	0.2307085102	-1.9393588365
Cl7	5.4828442057	3.2212455961	-0.9972746201
C8	3.0624323241	0.0926617497	1.4926704534
N9	4.4501888770	3.3254614642	2.6404267245
N10	6.0372821600	1.8641380697	2.2806683382
C11	3.2781398395	5.4051650403	2.0473855604
C12	2.0997114778	3.6153013988	3.2280450119
C13	2.6220138732	2.7439734336	-0.0946887928
C14	3.2484786927	4.1080121741	2.6004923972
C15	4.8489828152	2.3272612622	1.8197921118
C16	0.9435393138	4.3923099533	3.2957042758
C17	0.9484626746	5.6735111879	2.7409288319
C18	6.8128543855	0.7730167167	1.7503696163
C19	8.3021119878	-1.4140214413	0.8614602128
C20	6.4492699309	-0.5304862875	2.1157070673
C21	7.1824113258	-1.6279488499	1.6672730166
H22	2.7542759941	0.6136474898	2.3938973064
H23	3.7682036894	-0.7203087713	1.6236748315
H24	2.8184449874	3.7782235624	-0.3868013763
H25	0.0510479916	3.9991755546	3.7726466038
H26	6.8828174461	-2.6340925157	1.9444417755
C27	7.9699536351	1.0088333549	0.9778567705
C28	1.2422229934	2.3097665170	-0.0167365038
C29	8.6870607405	-0.1136559827	0.5354884195
C30	6.5551138546	2.6354046863	3.4313410908
C31	2.1020069430	6.1663623015	2.1266068449
C32	5.3570441176	3.5183638825	3.7967990769
C33	-1.1561052945	2.6275075020	-0.1580312803
C34	2.2767103325	0.1121398385	0.3488829168
H35	-0.4005312540	-0.6592059148	0.3976163265
H36	0.2905608147	4.2144043770	-0.3912738938
H37	-2.3501922663	0.8462444438	0.0859535950
H38	-2.0157336719	3.2744249353	-0.3074992219
C39	4.5185654461	5.9594605194	1.3902346111
C40	8.4659527813	2.3952784962	0.6500991436
H41	9.5653198143	0.0451609610	-0.0845198307
H42	6.8514471914	1.9573861925	4.2366220813
H43	2.0970591864	7.1657233327	1.6990945924
H44	5.6207546862	4.5737169525	3.9051365817
H45	5.3286114968	6.1015199272	2.1173559881
H46	4.3106016104	6.9336116983	0.9394353593
H47	7.6409817572	3.0718948261	0.4181163064
H48	9.1247235336	2.3661123500	-0.2216406988
H49	9.0487282770	2.8100401109	1.4842014110
H50	7.4294430578	3.2216858066	3.1293599118
C51	1.0460155081	0.9300014842	0.2134587831
H52	4.8953349267	5.2876548994	0.6109735918
H53	2.4283849408	-0.6625258261	-0.3973672500
H54	0.0558234524	6.2910619348	2.7869602074
H55	8.8788813561	-2.2567513704	0.4914280327
H56	5.5930159004	-0.6713857704	2.7666464991
H57	2.1174409211	2.6173462568	3.6564185771

5h

Ru1	0.0154852729	-0.0086303080	-0.0018839757
Cl2	0.0306103960	2.4485313773	-0.0907522306
N3	-2.9019614493	0.6075232957	0.0067647172
N4	-2.3578075571	0.0189363568	2.0425830504
C5	-1.8734506626	0.2312498340	0.7999903095
C6	-4.2129331550	0.5607028308	0.6873724529
H7	-4.8447497763	-0.2003288111	0.2159215374
H8	-4.7230523133	1.5249894454	0.6170173407
C9	-3.8259228682	0.2003599964	2.1307665121
H10	-4.0717173333	0.9948519197	2.8420801642
H11	-4.2911968481	-0.7283756940	2.4765260052
C12	-2.8351332849	0.8538193998	-1.4076519930
C13	-2.5612567590	-0.2169254943	-2.2678509845
C14	-2.5287043350	-0.0163073574	-3.6502077727
H15	-2.3087053322	-0.8499321537	-4.3105326749
C16	-2.7910814584	1.2521696905	-4.1679679000
C17	-3.0731752574	2.3127351058	-3.3034575450
H18	-3.2595844449	3.3024485250	-3.7128158992
C19	-3.0997859597	2.1452431252	-1.9125792987
C20	-3.3764046594	3.3235113774	-1.0104630062
H21	-4.4217455835	3.3445657432	-0.6740388800
H22	-3.1901585175	4.2605843327	-1.5423280364
H23	-2.7253892717	3.3006955810	-0.1327183856
C24	-1.6528843331	-0.4424183015	3.2035915713
C25	-1.2774126066	-1.7878978372	3.2805399868
C26	-0.6444773455	-2.2706017416	4.4270939625
H27	-0.3436342689	-3.3126385962	4.4785817460
C28	-0.3994215240	-1.4075175681	5.4979552759
C29	-0.7739351623	-0.0643978569	5.4113179673
H30	-0.5657594468	0.6066454125	6.2411540350
C31	-1.4034356377	0.4496622168	4.2674183763
C32	-1.7622968948	1.9156229618	4.1844143938
H33	-1.5735669352	2.3194053836	3.1851011637
H34	-1.1751670548	2.4954526097	4.9021651950
H35	-2.8202380329	2.0891837116	4.4206864716
C36	1.0158569927	-0.0048800460	1.5542668748
H37	0.6796050302	0.5232494764	2.4493076325
C38	2.3132077890	-0.6394749313	1.6272284364
C39	3.0223939743	-0.7903648753	2.8383449693
H40	2.6138501297	-0.3641573415	3.7506371688
C41	4.2128275255	-1.5103458959	2.8631579358
H42	4.7526107189	-1.6407122419	3.7965750105

C43	4.7081187068	-2.0810629883	1.6813654252
H44	5.6334626201	-2.6499520402	1.7043582441
C45	4.0268090762	-1.9213151939	0.4711785994
H46	4.4252929936	-2.3576745448	-0.4406902504
C47	2.8403981311	-1.1832155783	0.4291994605
C48	2.0790280993	-0.9496467033	-0.8181380593
H49	1.8003466969	-1.8317878544	-1.3884187536
C50	1.8830306106	0.2951231327	-1.3688124281
H51	2.3326350970	1.1904311636	-0.9540932565
H52	1.4651641852	0.3857460221	-2.3684259115
Cl53	-0.6059469483	-2.3714820404	-0.2512981959
H54	0.0881634527	-1.7752329133	6.3966764999
H55	-2.7726071098	1.4212394815	-5.2410651843
H56	-1.4563151398	-2.4314965333	2.4249120874
H57	-2.3697455836	-1.1981074782	-1.8459735865

5i

Ru1	0.0257366252	-0.0043931716	0.0025045404
Cl2	0.0123001568	2.4773009417	-0.0126446442
N3	-2.9360355508	0.2623638001	0.0123727731
N4	-2.2851360728	0.5541932395	2.0763671627
C5	-1.8562128908	0.2732052335	0.8301773982
C6	-4.1544860716	0.7707564598	0.6779115293
H7	-5.0218375931	0.1500936755	0.4429901526
H8	-4.3539199086	1.7944899190	0.3370812370
C9	-3.7557605189	0.7139757145	2.1563263449
H10	-4.0082294155	1.6250871145	2.7050739735
H11	-4.1979640886	-0.1425422650	2.6802440784
C12	-2.9184174090	0.0902843256	-1.4149679190
C13	-3.5372775005	-1.0451525568	-1.9819045803
C14	-3.5457016130	-1.1464709800	-3.3787135320
H15	-4.0047042236	-2.0188132542	-3.8369230315
C16	-2.9625144893	-0.1685781930	-4.1892782944
C17	-2.3544062765	0.9448637230	-3.6101427029
H18	-1.8995020145	1.7121094333	-4.2297188232
C19	-2.3405916031	1.0795436389	-2.2189601104
C20	-4.1384386039	-2.1355646556	-1.1295149125
H21	-5.0622432074	-1.8108731958	-0.6337743382
H22	-3.4290706790	-2.4516705168	-0.3592187729
H23	-4.3878268286	-3.0060115012	-1.7424058636
C24	-1.5235511770	0.5736811766	3.2908500578
C25	-1.3280147835	-0.6164396819	4.0208494236
C26	-0.6317964028	-0.5196133292	5.2352204165
H27	-0.4619013772	-1.4232426554	5.8152323963
C28	-0.1535152851	0.7048432392	5.7092078506
C29	-0.3584133700	1.8718849897	4.9689707300
H30	0.0191087386	2.8254444232	5.3257061749
C31	-1.0487845828	1.8031972779	3.7573704287
C32	-1.8190177828	-1.9507985314	3.5118742337
H33	-1.5268547145	-2.7522249640	4.1958522001
H34	-1.4112258963	-2.1805475978	2.5213874675
H35	-2.9123036329	-1.9740944289	3.4257887301
C36	1.1117018118	-0.0368153439	1.5022602453
H37	0.8354384417	0.4774411113	2.4240630777
C38	2.4020214870	-0.6889067797	1.4891619448
C39	3.1729107686	-0.8769719024	2.6568615910
H40	2.8191640789	-0.4678553312	3.5995962508
C41	4.3558774633	-1.6067812346	2.5993728020
H42	4.9438652037	-1.7650677188	3.4987548447
C43	4.7830866150	-2.1504600603	1.3787215650
H44	5.7038029457	-2.7258509715	1.3384753690
C45	4.0412179199	-1.9532519041	0.2108790559
H46	4.3883028597	-2.3667138298	-0.7320880869
C47	2.8619161897	-1.2034107035	0.2511200989
C48	2.0449646223	-0.9171317997	-0.9475476389
H49	1.7397366347	-1.7711299460	-1.5461116667
C50	1.8252956009	0.3540801685	-1.4264830980
H51	2.3011968659	1.2272187765	-0.9939097032
H52	1.3643171871	0.4910073434	-2.4014616976
Cl53	-0.5779698748	-2.3569122937	-0.2285019030
H54	0.3798019678	0.7452167784	6.6550833552
H55	-2.9822959099	-0.2819845125	-5.2696664709
H56	-1.8780462953	1.9409388070	-1.7475742625
H57	-1.1973029689	2.6875194637	3.1451347584

5j

Ru1	0.0207897153	0.0013724838	0.0032577337
Cl2	0.0241745083	2.4899670233	-0.0306404843
N3	-2.9408980731	0.3190656520	0.0120677788
N4	-2.2813036769	0.4746687109	2.0921925566
C5	-1.8597210889	0.2697043677	0.8241139484
C6	-4.1541418817	0.7748177885	0.7233269237
H7	-5.0324388770	0.2036032423	0.4161660070
H8	-4.3271151376	1.8360178169	0.5023691597
C9	-3.7606137449	0.5395019450	2.1814441948
H10	-4.0790742352	1.3432643023	2.8487997489
H11	-4.1411024128	-0.4140981186	2.5704754813
C12	-2.9406426444	0.2130960764	-1.4230201604
C13	-3.5466722702	-0.9098812433	-2.0280443560
C14	-3.5783452697	-0.9509714943	-3.4280000624
H15	-4.0299707783	-1.8111327865	-3.9155946425
C16	-3.0320211312	0.0742905481	-4.2048090069
C17	-2.4385277557	1.1752997248	-3.5879666678
H18	-2.0106652999	1.9782915312	-4.1808899787
C19	-2.4010452010	1.2494614237	-2.1930064496
C20	-4.1178315256	-2.0448852175	-1.2139047586
H21	-5.0240831332	-1.7444669408	-0.6663717499
H22	-3.3802406128	-2.4010592760	-0.4859206410
H23	-4.3925348197	-2.8826701033	-1.8645828513
C24	-1.5409051962	0.2291874868	3.2943629782
C25	-1.1812209625	-1.0837514590	3.6149367950
C26	-0.5132417485	-1.3509734247	4.8100053984
H27	-0.2257101008	-2.3686404906	5.0535531710
C28	-0.2178654657	-0.3028932146	5.6829390686
C29	-0.5773872117	1.0053081108	5.3526521938
H30	-0.3300584943	1.8168301876	6.0307518140
C31	-1.2422404315	1.3032565414	4.1540335658
C32	-1.5842395232	2.7263060148	3.7879451987
H33	-1.2743578624	2.9544018976	2.7614404002
H34	-1.0872579160	3.4242587342	4.4652195423
H35	-2.6617666875	2.9178171010	3.8583384438
C36	1.0974255066	0.0486836512	1.5083622958
H37	0.8231465093	0.6250826767	2.3941542949
C38	2.3819831766	-0.6134203077	1.5334456701
C39	3.1443493188	-0.7597584910	2.7119958830
H40	2.7903200638	-0.3080886150	3.6347779061
C41	4.3166424173	-1.5076896418	2.6920924501
H42	4.8967978528	-1.6365382378	3.6009315331
C43	4.7430861686	-2.1083828793	1.4981505312
H44	5.6553515458	-2.6980606281	1.4882479941
C45	4.0119767534	-1.9503767793	0.3184200672
H46	4.3589485061	-2.4077437452	-0.6040194468
C47	2.8425258231	-1.1840821051	0.3197592070
C48	2.0359420247	-0.9376914655	-0.8944597353
H49	1.7378799134	-1.8123670059	-1.4661573539
C50	1.8203450866	0.3167696791	-1.4223044904
H51	2.2943590887	1.2054717723	-1.0203481541
H52	1.3685744758	0.4153461164	-2.4064694550
Cl53	-0.5946871097	-2.3573757711	-0.1389057273
H54	0.2969547890	-0.5007633153	6.6189660444
H55	-3.0700574899	0.0081339594	-5.2886736875
H56	-1.4037101042	-1.8782625552	2.9099430773
H57	-1.9415185846	2.0953289269	-1.6928987551

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Ru1	0.0412755896	0.0455568759	0.0009237470
Cl2	0.0906746294	2.4792050768	-0.0533286713
Cl3	-2.3900851600	0.3016862922	-0.1040707106
N4	-0.3604671740	-1.8834827956	-2.2180736756
N5	-0.7984912158	-2.9736122586	-0.3720332432
C6	-0.3583108470	-1.7957427562	-0.8651394139
C7	-0.9430471909	-3.1474396242	-2.7157027820
H8	-0.2922317495	-3.5932789223	-3.4734019592
H9	-1.9257366490	-2.9613398487	-3.1627568917

C10	-1.0366179684	-3.9817271922	-1.4325398726
H11	-2.0139189743	-4.4527576057	-1.3006917438
H12	-0.2667993950	-4.7617910856	-1.3752032261
C13	0.1090297449	-0.8801254636	-3.1340914438
C14	1.4905712987	-0.8004904857	-3.3608297438
C15	2.0107908287	0.1189927459	-4.2700332455
H16	3.0826128804	0.1797331147	-4.4331951483
C17	1.1354121788	0.9551130831	-4.9669927664
C18	-0.2400188236	0.8560314036	-4.7576672438
H19	-0.9129706406	1.5116893377	-5.3035793739
C20	-0.7913359759	-0.0632872629	-3.8509113097
C21	-2.2874160527	-0.1578625063	-3.6811736634
H22	-2.6905280913	-1.0379734795	-4.2001236818
H23	-2.7738972404	0.7221303844	-4.1104472385
H24	-2.5684915444	-0.2155345801	-2.6257670162
C25	-0.8490497877	-3.4156099969	0.9931267398
C26	0.3272368597	-3.8826206399	1.5896582471
C27	0.3056424676	-4.4078184495	2.8812228621
H28	1.2246948720	-4.7551404842	3.3428713116
C29	-0.9069063703	-4.4721885111	3.5706668707
C30	-2.0809899308	-4.0203029822	2.9648081277
H31	-3.0211174177	-4.0778433958	3.5073559693
C32	-2.0866123897	-3.4930300762	1.6638765587
C33	-3.3749179892	-3.0421736699	1.0207142455
H34	-3.2770401884	-2.0388589677	0.5947313092
H35	-4.1858854523	-3.0316542536	1.7544254029
H36	-3.6769809327	-3.7215394030	0.2123079181
C37	-0.0576087174	-0.3178692334	1.8107235142
H38	-1.0046215036	-0.1256241704	2.3225686043
C39	1.0952251163	-0.7101340037	2.5940349524
C40	1.1042996425	-0.8195555140	3.9974371881
H41	0.2074129724	-0.5785829153	4.5615272105
C42	2.2619850651	-1.2447377844	4.6471457902
H43	2.2776968242	-1.3318953160	5.7296396619
C44	3.4064413608	-1.5647594523	3.9043588623
H45	4.3053954694	-1.8971813508	4.4162088211
C46	3.4079406365	-1.4501158618	2.5079052707
H47	4.3055091774	-1.6856839308	1.9418000458
C48	2.2576788686	-1.0119414943	1.8514372816
C49	2.1512233234	-0.8154457655	0.3785596120
H50	2.3102074450	-1.6918729684	-0.2471433327
C51	2.2486078553	0.4512439720	-0.1827610461
H52	2.4326809234	1.3198454717	0.4378618585
H53	2.4404747404	0.5815186411	-1.2431926820
H54	1.5224671544	1.6833977471	-5.6738224305
H55	2.1490285742	-1.4726812722	-2.8179210099
H56	1.2594874582	-3.8229756288	1.0363260971
H57	-0.9409760094	-4.8756036158	4.5788605617

5I

Ru1	0.0218736106	-0.0194932372	-0.0063911491
Cl2	0.0284945605	2.4403123367	-0.0947058042
N3	-2.9080613935	0.5228943516	0.0034566699
N4	-2.3524429919	0.0613457704	2.0664607223
C5	-1.8655230540	0.2323719503	0.8170617226
C6	-4.2128922244	0.3636085456	0.6801478386
H7	-4.6667377876	-0.5873156979	0.3726794405
H8	-4.8951478234	1.1767262148	0.4233074347
C9	-3.8007539638	0.3642706105	2.1526462791
H10	-3.9428347667	1.3428230690	2.6294108093
H11	-4.3192161066	-0.3920296797	2.7475992166
C12	-2.8603982745	0.6943398792	-1.4239067135
C13	-2.5953483599	-0.4097730695	-2.2420020274
C14	-2.5948858844	-0.2659806722	-3.6321694491
H15	-2.3808919895	-1.1245446874	-4.2618470563
C16	-2.8798063796	0.9770672804	-4.1964755065
C17	-3.1555422819	2.0715063068	-3.3721285863
H18	-3.3651326230	3.0399237556	-3.8190378657
C19	-3.1518318736	1.9611162182	-1.9757998358
C20	-3.4232621387	3.1665643556	-1.1095818707
H21	-4.3958606434	3.1005860284	-0.6048235088
H22	-3.4334500150	4.0772230544	-1.7146936274
H23	-2.6465449019	3.2707529826	-0.3464171500
C24	-1.6075907934	0.0146370708	3.2917788901
C25	-1.4348167477	-1.2122577915	3.9597705042
C26	-0.7561107016	-1.1867318875	5.1883505604
H27	-0.6004999854	-2.1221538721	5.7196371869
C28	-0.2796484979	0.0058634117	5.7377128349
C29	-0.4710284521	1.2145599855	5.0629236651
H30	-0.1000296462	2.1457729266	5.4805643084
C31	-1.1405087225	1.2154872459	3.8383494738
C32	-1.9457870261	-2.5069188584	3.3771021990
H33	-1.6591569370	-3.3521519310	4.0087617174
H34	-1.5507856659	-2.6721744706	2.3694092129
H35	-3.0403360798	-2.5069521694	3.2998548845
C36	1.0967600944	-0.0508009426	1.5004164188
H37	0.8207017264	0.4775087851	2.4141018429
C38	2.3776645263	-0.7213152747	1.5033623838
C39	3.1355153323	-0.9120113578	2.6790805510
H40	2.7813290673	-0.4884830533	3.6151715793
C41	4.3045392354	-1.6652547068	2.6387600579
H42	4.8816314268	-1.8261952298	3.5446776110
C43	4.7306795734	-2.2301000341	1.4273916265
H44	5.6398507397	-2.8243651434	1.4005477173
C45	4.0019832662	-2.0306523401	0.2516078844
H46	4.3476544274	-2.4616083104	-0.6840567577
C47	2.8373013735	-1.2576976038	0.2745730017
C48	2.0339835455	-0.9717290457	-0.9330891257
H49	1.7220252761	-1.8282358323	-1.5246194541
C50	1.8373433222	0.2965341271	-1.4286644201
H51	2.3211327305	1.1675899339	-1.0009040157
H52	1.3842307488	0.4322402028	-2.4072190171
Cl53	-0.5887473707	-2.3953125029	-0.1869687069
H54	0.2388327419	-0.0095641147	6.6924975344
H55	-2.8865468529	1.1000623918	-5.2759663391
H56	-2.3813398790	-1.3693341750	-1.7834175991
H57	-1.2822447487	2.1384093008	3.2828427874

b) M06-L optimized geometries

3a

N1	0.3100655054	0.3316094838	-0.6512650524
C2	1.7189778867	0.6555700416	-0.8789302962
C3	2.1114542908	-0.3796519786	-1.9185563837
N4	0.8089418905	-0.7782961383	-2.4650989774
C5	-0.4469350761	1.0140657846	0.3409739891
C6	-1.9801170281	2.3079009426	2.2673537574
C7	-1.4249786270	1.9305144032	-0.0482895312
C8	-0.2156049154	0.7239335169	1.6998779057
C9	-0.9970551709	1.3921796937	2.6452073791
C10	-2.1978006820	2.5753333824	0.9188844165
H11	-0.8511275453	1.1595991596	3.6987752464
H12	-2.9665166641	3.2799216616	0.6106647070
C13	-0.2246131571	-0.4167956968	-1.6613940899
Ru14	-2.1651503602	-0.6839056349	-1.7445410579
Cl15	-2.1638346528	-1.8050724001	0.4109094704
Cl16	-2.4565109380	1.1418108123	-3.3263952054
C17	-2.3514108423	-2.0809950049	-2.9464499858
H18	-1.5207975368	-2.6066125906	-3.4274294016
C19	0.7716277063	-1.7586469050	-3.4955968241
C20	0.7593991493	-3.6369862589	-5.5354639420
C21	0.8384918535	-3.1222567484	-3.1543977450
C22	0.6921687525	-1.3381885015	-4.8216823411
C23	0.6798992074	-2.2803938490	-5.8496814720
C24	0.8353200221	-4.0488000552	-4.2034598288
H25	0.6054969070	-1.9565738233	-6.8841050406
H26	0.8766768305	-5.1105121294	-3.9659295068
H27	2.7540737987	0.0173454220	-2.7102842592
H28	1.8073642823	1.6844866948	-1.2570776587
H29	2.2986149952	0.5809168835	0.0464000962
H30	2.6194794822	-1.2492044764	-1.4729481628
C31	-3.6627150696	-2.5121963177	-3.3538486340
C32	-6.2388695884	-3.2778366499	-4.1421574169
C33	-3.8489732573	-3.4729670073	-4.3653396929
C34	-4.8116075674	-1.9448844557	-2.7462192139
C35	-6.0940582341	-2.3267380054	-3.1300165770
C36	-5.1256136700	-3.8526129064	-4.7618146968
H37	-6.9699995525	-1.8927632281	-2.6592125379
H38	-7.2400401560	-3.5716922604	-4.4481006127
O39	-4.5180537861	-1.0188799735	-1.8063045585
C40	-5.5556240571	-0.4673017892	-0.9454679119
H41	-6.3825398418	-0.1601414563	-1.6031933651
H42	-2.9655359146	-3.9032073348	-4.8353527748
H43	-5.2595745175	-4.5901659281	-5.5479297162
C44	-4.9271392695	0.7442461496	-0.3001471060
H45	-4.0994511292	0.4344110718	0.3498016811
H46	-5.6662374517	1.2723930881	0.3102864216
H47	-4.5367524194	1.4290809712	-1.0607418559
C48	-5.9954868809	-1.5168631177	0.0538248310
H49	-5.1350195784	-1.8233756833	0.6575579513
H50	-6.4074523588	-2.4057957887	-0.4328167554
H51	-6.7641825232	-1.1054657477	0.7153684145
H52	-2.5803803810	2.8005461427	3.0284268647
H53	0.7548045445	-4.3803360933	-6.3291669885
H54	0.6114231543	-0.2735537973	-5.0263884501
C55	0.8080749798	-3.5519751589	-1.7189867145
H56	1.6351278321	-3.1287587807	-1.1354871849
H57	0.8618578510	-4.6400448275	-1.6305268792
H58	-0.1166179090	-3.2144205013	-1.2270067754
H59	-1.5736286357	2.1297384562	-1.1085877087
C60	0.7604956851	-0.3318265918	2.1143633723
H61	1.8017552688	0.0146733236	2.0810153953
H62	0.6747221342	-1.2046276205	1.4565691476
H63	0.5648302561	-0.6629679013	3.1375324566

3b

N1	0.3232486292	0.3868422357	-0.6997224975
C2	1.7498556056	0.6429285718	-0.8991719278
C3	2.1291626861	-0.4831007332	-1.8415190687
N4	0.8341035595	-0.8249879186	-2.4415666569
C5	-0.4257223933	1.0528269764	0.3076150274
C6	-1.9718714518	2.2907166261	2.2621712755
C7	-1.4293368136	1.9501615764	-0.0614204099
C8	-0.1736220373	0.7559605460	1.6618550097
C9	-0.9613805682	1.3977055534	2.6205993052
C10	-2.2098738749	2.5647768742	0.9184403776
H11	-0.7978736755	1.1600914934	3.6704598687
H12	-2.9979716826	3.2534481703	0.6233782990
C13	-0.2133632051	-0.3866654987	-1.6912590360
Ru14	-2.1571568276	-0.6498992270	-1.7634101035
Cl15	-2.0773484969	-1.8197667662	0.3544614603
Cl16	-2.6250319897	1.2264550412	-3.2604244287
C17	-2.3297665965	-2.0130586153	-3.0060430814
H18	-1.4907780207	-2.5289878664	-3.4827166642
C19	0.8000825136	-1.8198270692	-3.4572078461
C20	0.7742809451	-3.7799728937	-5.4192253515
C21	0.9909484750	-3.1570028721	-3.1041789024
C22	0.6075930861	-1.4290838040	-4.7932739238
C23	0.5945978713	-2.4399978503	-5.7624935209
C24	0.9756468079	-4.1449252802	-4.0870689121
H25	0.4387956164	-2.1631624725	-6.8038425195
H26	1.1115811445	-5.1880695097	-3.8153890913
H27	2.8450011647	-0.1863697494	-2.6147303657
H28	1.8907763692	1.6345508092	-1.3547558841
H29	2.2966770285	0.6194960952	0.0479557074
H30	2.5405039752	-1.3557104176	-1.3102345546
C31	-3.6367716770	-2.4361818072	-3.4343251195
C32	-6.2061604234	-3.1862470480	-4.2573201351
C33	-3.8150057544	-3.3521165399	-4.4879148950
C34	-4.7897165671	-1.9069186113	-2.8009072578
C35	-6.0689524623	-2.2834403970	-3.2010057488
C36	-5.0884049809	-3.7220639991	-4.9032491385
H37	-6.9484869538	-1.8820848640	-2.7083007823
H38	-7.2049301658	-3.4742749546	-4.5764098652
O39	-4.5041815479	-1.0253509796	-1.8167993582
C40	-5.5434231028	-0.5425013860	-0.9175816119
H41	-6.3854741311	-0.2219215894	-1.5489337160
H42	-2.9280865517	-3.7558006754	-4.9743565622
H43	-5.2162468036	-4.4233215293	-5.7229032926
C44	-4.9381709936	0.6503924649	-0.2179216455
H45	-4.0927336618	0.3319677198	0.4042783381
H46	-5.6827068771	1.1253093370	0.4285127426
H47	-4.5785787982	1.3835346902	-0.9477448547
C48	-5.9440105348	-1.6554794707	0.0277464779
H49	-5.0676637594	-1.9730493912	0.6024178043
H50	-6.3401361079	-2.5257429743	-0.5041036966
H51	-6.7134235128	-1.3017385175	0.7209822098
H52	-2.5762041777	2.7608533698	3.0341236879
H53	0.7596660617	-4.5409277557	-6.1960076749
H54	-1.5920187630	2.1595108177	-1.1168921350
C55	0.8348582808	-0.2743457005	2.0657422208
H56	1.8565963908	0.1260024276	2.1041592627
H57	0.8278456122	-1.1169366720	1.3653089935
H58	0.6096452708	-0.6660074681	3.0611015991
H59	1.1132888336	-3.4113213033	-2.0530584279
C60	0.3840961312	0.0069103743	-5.1487637510
H61	1.1532096771	0.6556119206	-4.7132515995
H62	-0.5769436118	0.3694427300	-4.7568297572
H63	0.3881883228	0.1512770836	-6.2323279088

3c

N1	0.3187390951	0.6381886341	-0.9697285031
C2	1.7778464608	0.5748015765	-0.8797677616
C3	2.1233494136	-0.3089672192	-2.0640493960
N4	0.8526132750	-0.9990690272	-2.3117161958
C5	-0.4290450933	1.4707650892	-0.0952290215
C6	-1.9601617612	3.0849720130	1.5728620532
C7	-0.3839385255	2.8665798772	-0.2744877101
C8	-1.2208457974	0.8917409699	0.8975743265
C9	-1.9931532295	1.7024468681	1.7307304702
C10	-1.1601973320	3.6526145072	0.5804976329

C11	0.3935652434	3.4872646948	-1.3936809302
H12	-2.6169865165	1.2489056739	2.4973221204
H13	-1.1610135727	4.7319734703	0.4373918244
H14	0.0141802426	4.4866165210	-1.6226735686
H15	0.3121234593	2.8812378521	-2.3032994698
C16	-0.2008989885	-0.3806204967	-1.7177385983
Ru17	-2.1215408334	-0.7647128944	-1.6685312858
Cl18	-1.8156030437	-2.5357724398	-0.0176059234
Cl19	-2.6728856111	1.4482610991	-2.4794388608
C20	-2.3908546050	-1.7784921666	-3.1953134675
H21	-1.6066856951	-2.0451423271	-3.9100319057
H22	1.4612637851	3.5957481742	-1.1600086069
C23	0.7826186149	-1.9342564323	-3.3806500609
C24	0.7237946939	-3.7787689577	-5.4487139596
C25	0.9245841875	-3.2905443253	-3.0983893908
C26	0.5946858728	-1.4659062485	-4.6942500881
C27	0.5750080423	-2.4173624336	-5.7202933524
C28	0.8896140171	-4.2202897868	-4.1365587349
H29	0.4224523986	-2.0823268214	-6.7448707677
H30	0.9866848304	-5.2806404110	-3.9196204401
C31	0.3205186403	-0.0152025933	-4.9534835063
H32	1.1423180081	0.6336846556	-4.6257947368
H33	-0.5736202023	0.3199013102	-4.4058348494
H34	0.1562810515	0.1715777424	-6.0177575894
H35	2.4203751079	0.2744059331	-2.9496508502
H36	2.2251477897	1.5718730919	-0.9374112367
H37	2.0698029005	0.1221791015	0.0791995744
H38	2.9173236619	-1.0317864086	-1.8531469666
C39	-3.7026054627	-2.2700395249	-3.5249858694
C40	-6.2769816595	-3.1912527718	-4.1317999050
C41	-3.9398258117	-3.0290929206	-4.6864717287
C42	-4.7977052811	-1.9936972495	-2.6675585313
C43	-6.0796948831	-2.4468770186	-2.9668164820
C44	-5.2151290398	-3.4894677851	-4.9901837619
H45	-6.9162788395	-2.2274464772	-2.3118980915
H46	-7.2780022256	-3.5448949921	-4.3666771653
O47	-4.4577442421	-1.2553886379	-1.5872414617
C48	-5.4178724758	-1.0043989733	-0.5208778520
H49	-6.3362342340	-0.6363418790	-1.0031507300
H50	-3.0956773295	-3.2485128560	-5.3389291576
H51	-5.3872562609	-4.0771368557	-5.8873963372
C52	-4.7920627874	0.0813454177	0.3201525572
H53	-3.8639325706	-0.2976237195	0.7663175927
H54	-5.4710159511	0.3710708143	1.1280513606
H55	-4.5492280370	0.9628796443	-0.2811235111
C56	-5.6662312726	-2.2784627879	0.2602621567
H57	-4.7225427944	-2.6270990107	0.6924726008
H58	-6.0722456598	-3.0806123611	-0.3619914557
H59	-6.3771240759	-2.0839002767	1.0694806989
H60	-1.2212319625	-0.1929827008	1.0098467370
H61	-2.5640891408	3.7249218587	2.2114607915
H62	0.6999640354	-4.4970948588	-6.2647587937
H63	1.0301698219	-3.5986616174	-2.0610105233

3d

N1	0.3138158093	0.6158521655	-0.9910229962
C2	1.7763812375	0.6387832975	-1.0171436631
C3	2.0699036573	-0.1633520254	-2.2698996834
N4	0.8391217748	-0.9476982712	-2.4211018002
C5	-0.4245956157	1.4244895521	-0.0854264535
C6	-1.9462515398	2.9847725297	1.6485865308
C7	-0.4391365008	2.8219994847	-0.2636772070
C8	-1.1555698980	0.8195711864	0.9385450123
C9	-1.9248339365	1.6012929869	1.8021136528
C10	-1.2059005122	3.5792976778	0.6257242490
C11	0.2574969225	3.4734228838	-1.4181461226
H12	-2.5019067706	1.1226664514	2.5897853393
H13	-1.2495139110	4.6579623414	0.4837754452
H14	-0.1896355067	4.4461444414	-1.6398252986
H15	0.1729842899	2.8544457297	-2.3183343493
C16	-0.2051964574	-0.4078098369	-1.7352934683
Ru17	-2.1263965368	-0.7951707148	-1.6452295117
Cl18	-1.9754504493	-2.5203691940	0.0884177830
Cl19	-2.6219571229	1.4048852008	-2.5045555779
C20	-2.3875674450	-1.8298062275	-3.1586604908
H21	-1.5929970842	-2.1142236972	-3.8555163509
H22	1.3244031469	3.6484580357	-1.2264037537
C23	0.7811358210	-1.9281025232	-3.4496621274
C24	0.7080054257	-3.8141981922	-5.4838912550
C25	0.8799087554	-3.2880317531	-3.1092231256
C26	0.6776101729	-1.5124088218	-4.7785001063
C27	0.6376802723	-2.4571085286	-5.8015876245
C28	0.8306959972	-4.2182761948	-4.1553019624
H29	0.5450916369	-2.1371844902	-6.8359968207
H30	0.8951835631	-5.2779476748	-3.9144814015
H31	2.2210526220	0.4766556052	-3.1531865206
H32	2.1593961833	1.6626334068	-1.0576387104
H33	2.1729869497	0.1578036329	-0.1102953331
H34	2.9378968979	-0.8241094624	-2.1749369261
C35	-3.7057862451	-2.2868748325	-3.5102875148
C36	-6.2963008619	-3.1180465924	-4.1743605634
C37	-3.9425567014	-3.0433987214	-4.6736437916
C38	-4.8103130510	-1.9658831926	-2.6799299941
C39	-6.1001877283	-2.3748576222	-3.0084884345
C40	-5.2260154139	-3.4591534116	-5.0059167565
H41	-6.9442501063	-2.1203834118	-2.3763077539
H42	-7.3039482334	-3.4352118983	-4.4320248064
O43	-4.4724199203	-1.2310130350	-1.5970525918
C44	-5.4572009595	-0.9118730555	-0.5711669569
H45	-6.3397234092	-0.5142411493	-1.0950177049
H46	-3.0919705645	-3.2924913107	-5.3067923313
H47	-5.3983073979	-4.0430232943	-5.9055236672
C48	-4.8134591613	0.1641317499	0.2690087919
H49	-3.9096837948	-0.2392344053	0.7428783492
H50	-5.5007330564	0.4892439782	1.0560893594
H51	-4.5266814291	1.0277982967	-0.3385883597
C52	-5.7931758784	-2.1548759176	0.2271128337
H53	-4.8859246746	-2.5313827552	0.7103382572
H54	-6.2044833346	-2.9549562559	-0.3942879338
H55	-6.5308681849	-1.9110302722	0.9980795821
H56	-1.1178557641	-0.2634097131	1.0487445817
H57	-2.5450888138	3.6029103954	2.3126783275
H58	0.6750267269	-4.5610968375	-6.2735484216
H59	0.5929297095	-0.4488156609	-4.9926302018
C60	1.0145438209	-3.7191896797	-1.6834840905
H61	1.8006966614	-3.1575606464	-1.1652841037
H62	1.2523928266	-4.7839399427	-1.6149570502
H63	0.0887466529	-3.5375140111	-1.1212105738

5a

Ru1	-0.2615848491	0.0731731266	0.0305075382
Cl2	-0.4964788982	2.5304121477	-0.0429251563
Cl3	-2.7585999777	0.0320175260	-0.0577294986
N4	-0.3759828265	-2.0120583583	-2.0577359866
N5	-0.8492408972	-3.0063759216	-0.1765362494
C6	-0.4839474305	-1.8301507905	-0.7187331413
C7	-0.9973826468	-3.2669614240	-2.4909191739
H8	-0.4184636410	-3.7526026519	-3.2806125767
H9	-2.0031940550	-3.0541936897	-2.8767195881
C10	-1.0305750007	-4.0586845307	-1.1922592034
H11	-1.9807140866	-4.5740504062	-1.0274751254
H12	-0.2201790717	-4.7979140983	-1.1286562814
C13	0.2132443835	-1.0571831341	-2.9266393772
C14	1.3475849674	-1.4163741228	-3.6861123034
C15	1.9505554004	-0.4137698975	-4.4551282173
H16	2.8337865447	-0.6670204917	-5.0395429720
C17	1.4730941189	0.8983483374	-4.4526335514
C18	0.3639642841	1.2364414906	-3.6779924473
H19	-0.0013103496	2.2583828867	-3.6407294872
C20	-0.2791961962	0.2516256683	-2.9269170291
C21	1.9369126055	-2.7961198377	-3.6545777064
H22	1.8435596529	-3.2619633973	-2.6660964627
H23	2.9996179932	-2.7677749990	-3.9113789468
H24	1.4571006480	-3.4706776924	-4.3756195358

C25	-0.8713069354	-3.3180496804	1.2132726157
C26	0.1451102959	-4.1274360456	1.7585826190
C27	0.0823636730	-4.4027576260	3.1302486439
H28	0.8693954801	-5.0086236698	3.5766325992
C29	-0.9357941130	-3.8855211242	3.9308062353
C30	-1.9190255637	-3.0685791115	3.3709563306
H31	-2.7044851804	-2.6453674069	3.9915534753
C32	-1.8920885480	-2.7891753288	2.0052985342
C33	1.2849784108	-4.6541615810	0.9377342696
H34	1.0467259713	-5.6172913771	0.4676866514
H35	2.1670789153	-4.8138751906	1.5647982363
H36	1.5687266878	-3.9586049649	0.1391138332
C37	-0.1391828292	-0.2992812796	1.8447584889
H38	-0.9882935530	-0.0394919112	2.4920522398
C39	1.0559834645	-0.8573282067	2.4265493607
C40	1.2303290561	-1.1559179985	3.7909871969
H41	0.4435066805	-0.9054767612	4.4996497116
C42	2.3891272319	-1.8067280476	4.2090492879
H43	2.5254474055	-2.0568978881	5.2580557363
C44	3.3711100340	-2.1617485251	3.2757196076
H45	4.2666490363	-2.6821431765	3.6080014364
C46	3.2193589753	-1.8453029338	1.9207338634
H47	3.9966179037	-2.1096332554	1.2053873530
C48	2.0746145439	-1.1726477229	1.4949639628
C49	1.8206942704	-0.7297412044	0.1083374999
H50	2.0518179739	-1.4404731860	-0.6898364556
C51	1.8022028689	0.6448034899	-0.2182378286
H52	2.0270523803	1.3971519613	0.5339868586
H53	1.9630188222	0.9557089097	-1.2494824760
H54	-1.1735687748	0.4912243490	-2.3457450437
H55	-2.6229081676	-2.1304973992	1.5357747684
H56	1.9803449377	1.6565672208	-5.0434119812
H57	-0.9485544448	-4.1054663940	4.9955707416

5b

C1	0.2784983892	0.0864036142	0.2074184995
C2	0.2231477138	2.9019718490	0.1454836979
C3	-0.9150374090	0.7826739129	0.4323525388
H4	4.3486092428	2.9117003836	4.7118301004
Ru5	4.3153812735	1.8197092147	-0.1577524115
Cl6	5.0715842650	0.9361729967	-2.2981102237
Cl7	5.6917835689	3.8526267500	-0.5108041091
C8	3.7152813694	-0.1751207950	0.6281242412
N9	4.2547026183	3.2440700788	2.6211723417
N10	5.7186937271	1.6436089561	2.4524361605
C11	3.1644204786	5.3075975232	1.9474851896
C12	1.8688513693	3.5353502245	3.0339390665
C13	2.7351658694	2.8152848495	-0.1981768246
C14	3.0735029296	4.0283086333	2.4977260418
C15	4.6965012838	2.2647224508	1.8103192597
C16	0.7632430636	4.3939737902	3.0365669566
C17	0.8471003656	5.6827692518	2.5065605337
C18	6.3893129946	0.4918497391	1.9675457245
C19	7.4801425473	-1.8268226014	0.8945009147
C20	6.3727652477	-0.6850933549	2.7447232734
C21	6.9401704458	-1.8338855581	2.1831395739
H22	3.4782299386	-0.1388915973	1.6913945668
H23	4.5201321244	-0.8516520132	0.3425256972
H24	2.8172755676	3.8939062566	-0.3839670096
H25	-0.1807297125	4.0329297479	3.4415824780
H26	6.9217013474	-2.7592292712	2.7566701326
C27	6.9503117634	0.5163234264	0.6884464590
C28	1.4353669558	2.2112298510	-0.0418628486
C29	7.4785823806	-0.6537054774	0.1415774104
C30	1.7648235209	2.1197998936	3.5127771341
C31	5.7208945352	-0.7396155182	4.0944285492
C32	6.1826127293	2.4046695266	3.6157784435
C33	2.0416236431	6.1353297606	1.9418889462
C34	4.9851447784	3.2931309661	3.8984410330
C35	-0.9430786854	2.1826911391	0.3953618763
C36	2.7759913366	0.2100323790	-0.3291701011
H37	0.2903353128	-1.0010908551	0.2171890044
H38	0.2156150540	3.9896940563	0.1292644348
H39	-1.8308405160	0.2301699876	0.6292457150
H40	-1.8802194137	2.7082900521	0.5619808787
H41	7.8667959926	-0.6404550946	-0.8724674868
H42	6.4450576562	1.7449388956	4.4468537454
H43	2.1024282419	7.1281464960	1.5050196460
H44	5.2578997218	4.3257050548	4.1345477901
H45	0.7496289092	1.8853407683	3.8440244969
H46	2.4476380871	1.9027326144	4.3441616676
H47	2.0203425562	1.4229519360	2.7020540803
H48	6.3938402840	-0.4071324828	4.8955503415
H49	5.4209571694	-1.7621386291	4.3399102384
H50	4.8271660325	-0.1046605355	4.1397657446
H51	7.0734688601	2.9822390743	3.3335299702
C52	1.4542561797	0.7979944442	-0.0257749480
H53	2.9225528346	-0.1493624813	-1.3496866449
H54	-0.0274371242	6.3286992037	2.5206370621
H55	7.8869431912	-2.7441437062	0.4769403376
H56	4.1109462862	5.6157317586	1.5069910124
H57	6.9591252998	1.4499179557	0.1224041337

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C1	0.1312320297	0.5865551634	0.2545400316
C2	0.3848308283	3.3553702599	-0.1842522376
C3	-0.9944448124	1.4198409691	0.2758052602
H4	4.4990024374	2.8939594391	4.6572191384
Ru5	4.3481412197	1.8297524392	-0.1319321774
Cl6	4.8962211682	0.7126440332	-2.2318199005
Cl7	5.9144636608	3.6683115632	-0.7327485540
C8	3.5223171088	0.0554767961	0.9240519619
N9	4.3831823029	3.3630866861	2.5981751112
N10	5.8856721472	1.7924805978	2.4036173852
C11	2.8723546492	5.2243219737	2.0922799272
C12	2.0261252088	3.1758718908	3.1301787373
C13	2.8898612974	2.9847692641	-0.2794275788
C14	3.0711326814	3.9211495128	2.5758790740
C15	4.8285700935	2.3779948533	1.7868776779
C16	0.7469450751	3.7195309092	3.2089973532
C17	0.5257384591	5.0135166278	2.7327297917
C18	6.4633528839	0.5637448192	1.9891754840
C19	7.3162618769	-1.9135109645	1.0532398926
C20	6.4348024164	-0.5401528121	2.8695770125
C21	6.8872726480	-1.7684272348	2.3747540321
H22	3.2580104446	0.2742893897	1.9583165354
H23	4.2571832221	-0.7358290346	0.7793567551
H24	3.0906613554	4.0359790433	-0.5294474388
H25	-0.0703492705	3.1355972685	3.6240669434
H26	6.8588091464	-2.6359729363	3.0322587871
C27	6.9104366018	0.4330312932	0.6722186745
C28	1.5269445600	2.5328671554	-0.1610146866
C29	7.3162510708	-0.8144016097	0.1966374082
C30	5.8782393840	-0.4515466034	4.2598494532
C31	6.3583631454	2.5935443391	3.5369593994
C32	1.5738707325	5.7480337716	2.1778926182
C33	5.1104403789	3.3810200177	3.8805406813
C34	-0.8698776827	2.7941572903	0.0417992779
C35	2.6503359176	0.3777321772	-0.1179736729
H36	0.0229436082	-0.4852960146	0.4057742729
H37	0.4950905957	4.4251264197	-0.3482944441
H38	-1.9763897907	0.9915309093	0.4635904845
H39	-1.7550601242	3.4257051625	0.0461327818
C40	4.0069235155	6.0030689064	1.5061662866
H41	7.6123095342	-0.9156414095	-0.8431685806
H42	6.7250677569	1.9653634039	4.3514007175
H43	1.3911242772	6.7530771371	1.8018465382
H44	5.3117903267	4.4087363130	4.1948766205
H45	4.7306350663	6.2953034171	2.2773301778
H46	3.6508256914	6.9176703017	1.0254344269
H47	6.6191614693	-0.0977008576	4.9884894803
H48	5.5449551315	-1.4343060535	4.6047084051
H49	5.0203725732	0.2301091692	4.3128831299
H50	7.1767028113	3.2426477342	3.1960720731

C51	1.3907315292	1.1385933364	0.0300082764
H52	4.5678125599	5.4099552101	0.7701489591
H53	2.7761429964	-0.1548936324	-1.0623983243
H54	-0.4701074638	5.4475514641	2.7843021306
H55	7.6296047578	-2.8898605305	0.6930092858
H56	2.2263458791	2.1658343972	3.4871481669
H57	6.9327646173	1.3105685867	0.0234928004

5d

Ru1	-0.2877519252	0.0986446830	-0.0662279191
Cl2	-0.6132707451	2.5410283578	-0.1997530790
Cl3	-2.7463092142	-0.0185268174	-0.4698545906
N4	-0.1057791654	-1.9585859836	-2.1725120684
N5	-0.7685527916	-2.9887624284	-0.3614146728
C6	-0.3504141605	-1.8001519317	-0.8505723394
C7	-0.6438438888	-3.2268122900	-2.6738698432
H8	0.0023020654	-3.6669954194	-3.4371297720
H9	-1.6346157967	-3.0454024465	-3.1119102969
C10	-0.7216441004	-4.0397477836	-1.3947793705
H11	-1.6096556344	-4.6752512774	-1.3350949447
H12	0.1681100790	-4.6697780631	-1.2382339647
C13	0.5538261452	-0.9858768019	-2.9686788561
C14	1.7811673578	-1.3196406356	-3.5815924661
C15	2.4493478577	-0.3048098575	-4.2765153929
H16	3.4038449080	-0.5369339690	-4.7462879310
C17	1.9423567326	0.9949499459	-4.3402877073
C18	0.7383921450	1.3071958876	-3.7099725063
H19	0.3467693243	2.3199500573	-3.7246648828
C20	0.0320999613	0.3091812211	-3.0364503680
C21	2.3948726130	-2.6841023321	-3.4645546072
H22	2.2108159892	-3.1341768585	-2.4810914769
H23	3.4772229984	-2.6345117815	-3.6121019110
H24	2.0068705818	-3.3845208287	-4.2156092185
C25	-0.6075106221	-3.3932477188	1.0020934759
C26	0.6687053545	-3.7972731851	1.4059742728
C27	0.8873057187	-4.2408630152	2.7072809010
H28	1.8848630629	-4.5326283912	3.0253704111
C29	-0.1843416032	-4.2725346807	3.6019117154
C30	-1.4562885497	-3.8795088931	3.1871043967
H31	-2.2879321120	-3.9109883494	3.8885634137
C32	-1.7049542583	-3.4450026340	1.8755567549
C33	-3.0763339869	-3.0573943594	1.4267043250
H34	-3.0888330892	-2.0524894392	0.9857918871
H35	-3.7855565927	-3.0887655270	2.2575092330
H36	-3.4447988138	-3.7339587961	0.6459003023
C37	-0.3902053062	-0.2838015305	1.7481035701
H38	-1.3562802035	-0.1460823050	2.2546946236
C39	0.7671117400	-0.6736242805	2.5143801735
C40	0.7808734678	-0.9076801682	3.9025191354
H41	-0.1259091278	-0.7510480265	4.4833253892
C42	1.9483172750	-1.3635026664	4.5107407990
H43	1.9645057074	-1.5576413755	5.5802689879
C44	3.0982624380	-1.5929019635	3.7452791191
H45	4.0016096550	-1.9602339311	4.2272159471
C46	3.0983639439	-1.3535176113	2.3668280113
H47	3.9985047066	-1.5266584401	1.7796101005
C48	1.9416214326	-0.8768311591	1.7519244606
C49	1.8241066385	-0.5561373925	0.3139663945
H50	2.1769229481	-1.3125986463	-0.3926709490
C51	1.7656958377	0.7828644000	-0.1185210840
H52	1.8533801795	1.5976478060	0.5957803967
H53	2.0219418742	1.0356553801	-1.1464866106
H54	2.4997173231	1.7642218528	-4.8683620650
H55	-0.9299651398	0.5285960709	-2.5670776735
H56	-0.0269799338	-4.5996664887	4.6270071255
H57	1.4917966818	-3.7382372433	0.6935405756

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C1	0.4700842074	-0.1500872280	0.1174360805
C2	0.1064367001	2.6301440293	0.3865303564
C3	-0.7783850507	0.3772503207	0.4660256109
H4	4.7461467216	3.6346397535	4.6848742544
Ru5	4.2699955473	2.0688009532	-0.2122598827
Cl6	4.8621512539	1.5720943186	-2.5252638267
Cl7	5.3774317330	4.2754349168	-0.3981035342
C8	3.9287561963	-0.0438732640	0.3862772783
N9	4.3442091338	3.2795259464	2.6365602292
N10	5.8914793130	1.7707562245	2.3360002777
C11	3.1393442962	5.3465938285	2.1566875630
C12	1.9718798133	3.4171873936	3.1138797390
C13	2.5916420564	2.8683370097	-0.0492319169
C14	3.1324721080	4.0214694685	2.5942379177
C15	4.7907446198	2.3451770937	1.7781908251
C16	0.8132181089	4.1987629722	3.1891072785
C17	0.8075093897	5.5252237012	2.7542422269
C18	6.4357107060	0.4889383092	2.0084746471
C19	7.4200309161	-2.0653925460	1.4974862079
C20	6.1150275913	-0.5770912532	2.8614698952
C21	6.6019589608	-1.8549598156	2.6115050551
H22	3.7349539719	-0.1377329827	1.4535663669
H23	4.7871572427	-0.6034511404	0.0142861726
H24	2.5455958822	3.9621774774	-0.1209635337
H25	-0.0985810298	3.7500858839	3.5797454141
H26	6.3377854592	-2.6781941553	3.2698604214
C27	7.2713263040	0.3036137024	0.8966097474
C28	1.3766799210	2.1052557580	0.0801448602
C29	7.7429096854	-1.0001091899	0.6611791027
C30	1.9807110151	1.9755335101	3.5203918925
C31	6.1854231655	2.3156860886	3.6722258578
C32	1.9666259987	6.0978567473	2.2262011906
C33	5.2830339707	3.5330517152	3.7360571514
C34	-0.9613869966	1.7605913160	0.5910985299
C35	2.9080238495	0.3131437764	-0.4941475873
H36	0.5997010188	-1.2233540921	-0.0011340018
H37	-0.0203085827	3.7052882519	0.4902743358
H38	-1.6178722795	-0.2940697486	0.6308491591
H39	-1.9420769462	2.1542302674	0.8463924888
C40	7.6238582369	1.4173023025	-0.0357805671
H41	8.3812463020	-1.1682260547	-0.2038844931
H42	5.9428630529	1.5714486088	4.4436113120
H43	1.9598094918	7.1235316027	1.8682023805
H44	5.8225391025	4.4696897416	3.5389391215
H45	1.0067633950	1.6631893282	3.9063418309
H46	2.7377320674	1.7668276167	4.2875546084
H47	2.2213711912	1.3346223542	2.6604207332
H48	6.9421115016	1.4542848686	-0.8991856024
H49	8.6269131062	1.2743456747	-0.4482740961
H50	7.5699498340	2.3998950520	0.4406793816
H51	7.2498998784	2.5544378159	3.7533073887
C52	1.5491051343	0.7114813371	-0.0734860962
H53	3.0350847089	0.0656426929	-1.5494387094
H54	-0.1068416571	6.1098780917	2.8194841475
H55	7.8064845797	-3.0587665975	1.2841221706
H56	4.0536294548	5.7516442549	1.7291486481
H57	5.4515303647	-0.4003389232	3.7067029461

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Ru1	-0.6645672743	0.0071515223	-0.0065608625
Cl2	-1.4692244153	2.3278621606	0.4109936289
Cl3	-3.0688374429	-0.6239077283	-0.0817035393
N4	-0.1966483616	-2.0321118493	-2.2200958234
N5	-0.6686897316	-3.0556445747	-0.3426237198
C6	-0.4293439726	-1.8496046785	-0.8873952795
C7	-0.2247097298	-3.4613541156	-2.5829424318
H8	0.7930085385	-3.8398019483	-2.7462406157
H9	-0.7963152321	-3.6053625817	-3.5035292256
C10	-0.8676075644	-4.0913612135	-1.3627772638
H11	-1.9460694785	-4.2546694755	-1.4919427326
H12	-0.4080519587	-5.0371369571	-1.0613521440
C13	0.5391977956	-1.1229868275	-3.0429691337
C14	1.8027565007	-1.5326366899	-3.4977119873
C15	2.5748001477	-0.7021860257	-4.3027910058
H16	3.5526630192	-1.0340826401	-4.6414712138
C17	2.0827483717	0.5544743076	-4.6614772943

C18	0.8293800762	0.9569694201	-4.2087549410
H19	0.4420948959	1.9338096533	-4.4916134627
C20	0.0265531380	0.1364122661	-3.3981221464
C21	-1.3064617615	0.6223967691	-2.9277008334
H22	-1.9893890369	-0.1899271860	-2.6648230612
H23	-1.7868198695	1.2422747959	-3.6906083693
H24	-1.2282184925	1.2828730666	-2.0456534289
C25	-0.5668658157	-3.3928646604	1.0376043180
C26	0.6521378532	-3.9450955500	1.4816074142
C27	0.7589271449	-4.2673829195	2.8388896756
H28	1.6985507525	-4.6727484760	3.2104993456
C29	-0.3009590409	-4.0444433286	3.7200068659
C30	-1.4945262464	-3.4898207461	3.2569431987
H31	-2.3162024346	-3.3001023162	3.9425797064
C32	-1.6330492587	-3.1660880855	1.9062831358
C33	1.8037461368	-4.1485719085	0.5421181159
H34	1.6518119034	-5.0125249070	-0.1184767529
H35	2.7323135935	-4.3206385391	1.0926905414
H36	1.9563080355	-3.2751454429	-0.1056066564
C37	-0.4069540128	-0.3970303057	1.7879926996
H38	-1.2813275565	-0.3454232296	2.4507739050
C39	0.8954130479	-0.6521192750	2.3387047672
C40	1.1672571059	-0.9314229662	3.6922292472
H41	0.3571715592	-0.9075160053	4.4180958491
C42	2.4616515900	-1.2734300874	4.0731006468
H43	2.6811106779	-1.5057387046	5.1119235034
C44	3.4820283660	-1.3419807068	3.1142479450
H45	4.4872325328	-1.6245130882	3.4187215809
C46	3.2286128782	-1.0367884577	1.7729862132
H47	4.0325572245	-1.0709145544	1.0396207288
C48	1.9418678826	-0.6615150283	1.3857503150
C49	1.5582948633	-0.2539513845	0.0220034873
H50	1.9583587941	-0.8558180107	-0.7971358983
C51	1.1803553384	1.0779240070	-0.2680116444
H52	1.2283854297	1.8508842883	0.4953090480
H53	1.2543643118	1.4324831660	-1.2965551331
H54	2.6712384428	1.2135628487	-5.2941845942
H55	-0.1862051681	-4.2906110633	4.7729385896
H56	-2.5319923053	-2.6940000297	1.5114315755
H57	2.1943695608	-2.5034729332	-3.2048734838

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C1	0.3650035891	0.3873583496	0.2054660499
C2	0.3373258296	3.1959810041	0.0192648078
C3	-0.8260373732	1.1035570451	0.3776993813
H4	4.8035983595	3.0879634465	4.5666368384
Ru5	4.4220519881	2.0681071634	-0.2652069348
Cl6	5.1049251393	1.0856672980	-2.3765718916
Cl7	5.7248804158	4.1047926246	-0.8214687774
C8	3.8085909883	0.1400131551	0.6644062111
N9	4.4956040465	3.4723598060	2.5126569010
N10	6.1556102408	2.0857811651	2.1336349841
C11	2.7734749502	5.2030220194	2.2496392535
C12	2.2177245268	3.0061303986	3.1732666869
C13	2.8536330607	3.0823607911	-0.2459515019
C14	3.1377117525	3.8958432133	2.6093566793
C15	4.9734395719	2.5553990214	1.6463923571
C16	0.9011005581	3.4040690867	3.3856827797
C17	0.5163724072	4.6999807257	3.0351421753
C18	6.5656567509	0.7216927581	1.9700536958
C19	7.1443047405	-1.9834627073	1.7177609023
C20	6.0913647458	-0.1916660902	2.9210032451
C21	6.3823064524	-1.5469856773	2.8049601718
H22	3.5700429189	0.2497384110	1.7210221552
H23	4.6103451685	-0.5601232493	0.4304403894
H24	2.9366162930	4.1633122253	-0.4239278253
H25	0.1815585646	2.7080814395	3.8087571949
H26	6.0031625763	-2.2542006581	3.5378665660
C27	7.3816696024	0.3137213197	0.9044261362
C28	1.5481768861	2.4885196489	-0.1042940159
C29	7.6341654083	-1.0640477554	0.7915658874
C30	6.5943591553	2.8588827663	3.3057095127
C31	1.4400358919	5.5794288272	2.4701374609
C32	5.3231291132	3.5755536951	3.7270325935
C33	-0.8419968581	2.4989451639	0.2708087982
C34	2.8662696629	0.4595923509	-0.3125925536
H35	0.3632086635	-0.6992190181	0.2590221157
H36	0.3386667729	4.2818199814	-0.0465449058
H37	-1.7493630113	0.5677770437	0.5857865434
H38	-1.7772404726	3.0396630010	0.3948279193
C39	3.7744600984	6.1371758495	1.6481241443
C40	7.9852385350	1.2931857734	-0.0510257637
H41	8.2360875599	-1.4108520515	-0.0456031597
H42	6.9984727971	2.1941834458	4.0741574466
H43	1.1294888961	6.5846712236	2.1911942104
H44	5.4848490673	4.6251173191	3.9892312908
H45	4.5083559921	6.4711279680	2.3922820155
H46	3.2887971864	7.0290666148	1.2444163274
H47	7.2479743517	1.9531223489	-0.5216082701
H48	8.5185111058	0.7764338649	-0.8518589270
H49	8.6917624695	1.9522114579	0.4678429749
H50	7.3807963679	3.5597466773	2.9974917103
C51	1.5512238683	1.0766154759	-0.0383273619
H52	4.3481552557	5.6505279380	0.8470626975
H53	3.0012457703	0.0283586184	-1.3061093119
H54	-0.5100832630	5.0224093226	3.1932452806
H55	7.3625678496	-3.0413846264	1.5961165754
H56	5.4637905518	0.1750947391	3.7341262501
H57	2.5472272145	2.0004521360	3.4334528402

5h

Ru1	-0.0831921701	-0.0406581110	0.0560452989
Cl2	-0.2973168130	2.4626015226	0.0999237851
N3	-2.9802351716	0.4771129559	0.0035074673
N4	-2.5084877227	-0.1460488319	2.0419936079
C5	-1.9863118465	0.1067058832	0.8349591540
C6	-4.3030862613	0.3411269517	0.6233774690
H7	-4.8138692305	-0.5361165854	0.2043531727
H8	-4.9245071620	1.2221897834	0.4380157687
C9	-3.9468705849	0.1614590114	2.0983709518
H10	-4.1126310724	1.0774689795	2.6823100197
H11	-4.4937766921	-0.6564944941	2.5764703602
C12	-2.7350174390	0.8082505236	-1.3592177185
C13	-2.0415407283	-0.1080723798	-2.1586374432
C14	-1.6535133973	0.2449573666	-3.4535706188
H15	-1.1016293956	-0.4669280552	-4.0627192384
C16	-1.9854985880	1.5027884465	-3.9521896819
C17	-2.6940190636	2.4020655714	-3.1522498633
H18	-2.9187687667	3.3971917108	-3.5317178550
C19	-3.0713008255	2.0880239825	-1.8422457576
C20	-3.7047192909	3.1174513503	-0.9596019558
H21	-4.7867910366	2.9711098635	-0.8468531268
H22	-3.5550559910	4.1198323241	-1.3689020190
H23	-3.2484474701	3.0945505688	0.0377920244
C24	-1.7206222301	-0.4182140685	3.1995183648
C25	-1.2479737614	-1.7167884455	3.3943792655
C26	-0.4148190698	-1.9945867963	4.4774867730
H27	-0.0259887249	-2.9998541841	4.6154720702
C28	-0.0713064777	-0.9718902055	5.3628456574
C29	-0.5426714770	0.3254060109	5.1528555943
H30	-0.2426612533	1.1263876732	5.8260680819
C31	-1.3666772489	0.6360835684	4.0624651156
C32	-1.7748467166	2.0484485491	3.7740991070
H33	-1.6117032194	2.2996899641	2.7167739764
H34	-1.1935039871	2.7514591889	4.3758195729
H35	-2.8332206463	2.2313166513	3.9976380292
C36	1.0079148804	-0.0591973994	1.5622943673
H37	0.7432194589	0.4721490176	2.4871718947
C38	2.2673049208	-0.7514780009	1.5228745299
C39	3.0563265946	-1.0119994456	2.6629224857
H40	2.7417592585	-0.6186246249	3.6277612672
C41	4.1960345118	-1.7997433644	2.5490430075
H42	4.7985469367	-2.0196736224	3.4263279919
C43	4.5625040059	-2.3280505166	1.3024933593

H44	5.4511660373	-2.9496030138	1.2216170858
C45	3.8052893292	-2.0579545801	0.1614275596
H46	4.1058776624	-2.4582366479	-0.8043825821
C47	2.6708318286	-1.2488626850	0.2556534576
C48	1.8431859770	-0.8627341189	-0.8946959666
H49	1.5739855199	-1.6511879326	-1.5970472416
C50	1.6422304176	0.4681099190	-1.2562095857
H51	2.1566477352	1.2841208025	-0.7540575258
H52	1.2210471027	0.7074108755	-2.2307756855
Cl53	-0.6006398220	-2.4931077870	-0.0169370524
H54	0.5817373251	-1.1785460831	6.2075248286
H55	-1.6848969395	1.7935155924	-4.9555972714
H56	-1.4972027776	-2.4795222572	2.6606021266
H57	-1.8223647532	-1.0997246841	-1.7636135245

5i

Ru1	-0.0513429430	0.0984082132	0.0556835699
Cl2	-0.0638173927	2.6082969031	0.3077041836
N3	-3.0051345152	0.2636614783	0.0305393767
N4	-2.3896666867	0.5724083265	2.0979329213
C5	-1.9445168545	0.3208044242	0.8615583284
C6	-4.2538578114	0.6560578060	0.6963664668
H7	-5.0703198843	-0.0274920895	0.4463913655
H8	-4.5371979367	1.6663894307	0.3723036323
C9	-3.8583203569	0.6044090695	2.1700006803
H10	-4.1952257267	1.4762802930	2.7389344562
H11	-4.2255650847	-0.3003735049	2.6764875021
C12	-2.8663472745	0.0354939244	-1.3674168046
C13	-3.4984469492	-1.0758722395	-1.9586958129
C14	-3.2414419883	-1.3190918730	-3.3117916827
H15	-3.6977672684	-2.1902079213	-3.7783282085
C16	-2.3689755505	-0.5175119796	-4.0508543657
C17	-1.7399378106	0.5671121391	-3.4434998026
H18	-1.0576690071	1.1986324151	-4.0071696642
C19	-1.9997182711	0.8540537660	-2.1007719098
C20	-4.3135500797	-2.0347710791	-1.1482442498
H21	-5.3285949179	-1.6685585256	-0.9474865347
H22	-3.8228737819	-2.2291187137	-0.1862553511
H23	-4.4126651423	-2.9908454600	-1.6687808288
C24	-1.5591376639	0.5893094280	3.2553848560
C25	-1.1698039545	-0.6289426260	3.8423089488
C26	-0.2935090088	-0.5642766811	4.9339463088
H27	0.0347690342	-1.4931158923	5.3973504566
C28	0.1827297784	0.6582284527	5.4118576341
C29	-0.2126269466	1.8530586067	4.8069575727
H30	0.1736874236	2.8047343396	5.1607975995
C31	-1.0903771179	1.8168130794	3.7234200868
C32	-1.6029365119	-1.9381876059	3.2617479586
H33	-1.2986746426	-2.7727561644	3.8984890805
H34	-1.1641896817	-2.0918581612	2.2645486539
H35	-2.6899751038	-1.9941724819	3.1279657477
C36	1.0611008013	-0.0028497264	1.5438738681
H37	0.8382522718	0.5443167748	2.4686731871
C38	2.3085335834	-0.7144889980	1.4818291018
C39	3.1079522973	-0.9842634280	2.6124897186
H40	2.8035223861	-0.5965813282	3.5833182995
C41	4.2512163522	-1.7632467818	2.4780387631
H42	4.8657711050	-1.9870235676	3.3460315980
C43	4.6084972210	-2.2726409597	1.2211334033
H44	5.5014993606	-2.8854647003	1.1238926992
C45	3.8392850971	-1.9924594526	0.0898661441
H46	4.1368431096	-2.3760767574	-0.8835012985
C47	2.7004170353	-1.1915772450	0.2050016059
C48	1.8611915598	-0.7852494290	-0.9311167071
H49	1.5460035998	-1.5675700615	-1.6203956576
C50	1.6794392901	0.5458332174	-1.2921383660
H51	2.2184604147	1.3559571116	-0.8063159178
H52	1.2411135612	0.7788535742	-2.2613315657
Cl53	-0.7474664485	-2.2545269988	-0.3494564616
H54	0.8731868553	0.6767637134	6.2518749090
H55	-2.1719004750	-0.7529174402	-5.0936039027
H56	-1.5460782762	1.7182409067	-1.6145423747
H57	-1.3719063369	2.7222716359	3.1918194368

5j

Ru1	-0.0577712458	0.1322736286	0.0614279124
Cl2	-0.0528336843	2.6519502037	0.2880677263
N3	-3.0099174691	0.3524242884	0.0360164913
N4	-2.3958529237	0.4365804785	2.1276738351
C5	-1.9509793399	0.3292821209	0.8679408292
C6	-4.2599358168	0.6501532326	0.7470008047
H7	-5.0814676981	0.0209789737	0.3944589792
H8	-4.5306771268	1.7019234856	0.5811109490
C9	-3.8658113876	0.3729193635	2.1932959032
H10	-4.2603685165	1.1104325962	2.8988806899
H11	-4.1691381454	-0.6294163632	2.5308725446
C12	-2.8761704891	0.1793659430	-1.3714931238
C13	-3.4895716287	-0.9230221693	-1.9995061412
C14	-3.2359343574	-1.1107522630	-3.3623993351
H15	-3.6819795860	-1.9703528613	-3.8592248778
C16	-2.3861612940	-0.2640784539	-4.0771020634
C17	-1.7756679376	0.8100279653	-3.4331666560
H18	-1.1115089814	1.4780929131	-3.9759337671
C19	-2.0302233567	1.0401827586	-2.0790853104
C20	-4.2987053152	-1.9185621137	-1.2281273965
H21	-5.3253332703	-1.5771967160	-1.0416326663
H22	-3.8254543844	-2.1293873132	-0.2615920143
H23	-4.3687026328	-2.8624052605	-1.7748423935
C24	-1.5735198786	0.2081154684	3.2680470855
C25	-1.0836564582	-1.0798722076	3.4981527956
C26	-0.2122692960	-1.3058383500	4.5629988523
H27	0.1935339842	-2.3001397564	4.7304709855
C28	0.1526954874	-0.2413213982	5.3900102987
C29	-0.3454399707	1.0408263738	5.1495214468
H30	-0.0384073690	1.8696333631	5.7846644205
C31	-1.2143482678	1.2972153246	4.0798244834
C32	-1.6766998209	2.6825070684	3.7520235346
H33	-1.3465047854	2.9640869884	2.7425433956
H34	-1.2762592537	3.4104812335	4.4619662104
H35	-2.7699471912	2.7675541399	3.7675470692
C36	1.0600002970	0.0753795544	1.5465139991
H37	0.8427283600	0.6524892230	2.4554646365
C38	2.2992578048	-0.6500079790	1.4992640499
C39	3.1056200420	-0.8986564395	2.6297207845
H40	2.8169312362	-0.4777007666	3.5915172010
C41	4.2314871948	-1.7044504266	2.5084207225
H42	4.8494252503	-1.9148761753	3.3774405511
C43	4.5653743763	-2.2597872948	1.2642835258
H44	5.4440176267	-2.8946462705	1.1781409249
C45	3.7915009811	-1.9977487505	0.1319845156
H46	4.0708952928	-2.4169871265	-0.8319803388
C47	2.6700181614	-1.1707780341	0.2333628875
C48	1.8252500564	-0.7814250229	-0.9045339614
H49	1.5071262413	-1.5748598199	-1.5795868980
C50	1.6568844252	0.5457015666	-1.2967847589
H51	2.2104551953	1.3596188227	-0.8340656269
H52	1.2218091714	0.7599665245	-2.2716876984
Cl53	-0.7854112039	-2.2250465259	-0.2005655852
H54	0.8375767809	-0.4059475635	6.2188180651
H55	-2.1942026126	-0.4543266937	-5.1299968559
H56	-1.3442470885	-1.8747168778	2.7999573609
H57	-1.5874351865	1.8911781783	-1.5637512424

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Ru1	-0.6071963558	0.1115658653	-0.0201559137
Cl2	-1.2122131423	2.5008982639	0.2853916959
Cl3	-3.0520643742	-0.2662568128	-0.2081209891
N4	-0.4652816408	-1.8666231048	-2.2634701719
N5	-0.8304995570	-2.9658496688	-0.3934065186
C6	-0.5491326834	-1.7493448770	-0.9072980545
C7	-0.9384623383	-3.1903266024	-2.7011063763
H8	-0.3300514156	-3.5734295084	-3.5238021184
H9	-1.9749908366	-3.0933587710	-3.0477382304
C10	-0.8443577976	-4.0128129434	-1.4295842300

H11	-1.6970031773	-4.6821683699	-1.2841830773
H12	0.0790798356	-4.6091938485	-1.3608232833
C13	0.4866168204	-1.1379427684	-3.0462333589
C14	1.6733008879	-1.8091704762	-3.3828233215
C15	2.6573746818	-1.1746600942	-4.1321986283
H16	3.5748388003	-1.6994793301	-4.3849773737
C17	2.4547431611	0.1471263732	-4.5412745253
C18	1.2771608572	0.8073247356	-4.2015882473
H19	1.1237462223	1.8354763367	-4.5240945412
C20	0.2615826536	0.1850498282	-3.4530688597
C21	-0.9831222180	0.9302849050	-3.0903163923
H22	-1.7894079544	0.2667905514	-2.7625479241
H23	-1.3480346871	1.5212111968	-3.9361670288
H24	-0.8105482461	1.6530625920	-2.2772036597
C25	-0.5075629428	-3.3707644203	0.9405086735
C26	0.8384962539	-3.6430568001	1.2073353868
C27	1.2288898128	-4.1010417089	2.4620200046
H28	2.2782757180	-4.2899531757	2.6727010069
C29	0.2581649797	-4.2818446874	3.4492952737
C30	-1.0830901551	-4.0232575990	3.1697350844
H31	-1.8355059887	-4.1752870949	3.9412304268
C32	-1.5038293945	-3.5783343393	1.9061757421
C33	-2.9469195669	-3.3399413642	1.6034328390
H34	-3.1282955595	-2.3014052711	1.2988504053
H35	-3.5723792722	-3.5729340996	2.4684142477
H36	-3.2863420883	-3.9575488149	0.7634416379
C37	-0.4463813590	-0.3316414314	1.7751460988
H38	-1.3576581823	-0.2968154490	2.3891573049
C39	0.8226948534	-0.6067061104	2.3947206072
C40	1.0184936955	-0.8799429552	3.7624129350
H41	0.1717648071	-0.8440548286	4.4447352282
C42	2.2889948840	-1.2231123983	4.2178149332
H43	2.4482867587	-1.4476640793	5.2693299671
C44	3.3620493680	-1.2998042636	3.3199925744
H45	4.3483847255	-1.5801673278	3.6828403069
C46	3.1811103947	-1.0156822145	1.9622600410
H47	4.0222960473	-1.0660133082	1.2733251124
C48	1.9178458998	-0.6473037533	1.4998753168
C49	1.6038155026	-0.2932790716	0.1018322096
H50	1.9647086683	-0.9734422690	-0.6734739412
C51	1.3305462467	1.0400757937	-0.2625112013
H52	1.3989436302	1.8403467425	0.4700296588
H53	1.4534283968	1.3469186479	-1.3011783512
H54	3.2150770588	0.6595291802	-5.1249799480
H55	1.8190901648	-2.8315412969	-3.0343491903
H56	1.5755692799	-3.4731517330	0.4223085563
H57	0.5476431504	-4.6239187905	4.4400247680

5l

Ru1	-0.1040806652	-0.0888471830	0.0473086667
Cl2	-0.3627333146	2.4077792528	0.1061360261
N3	-3.0085800031	0.3713721862	-0.0043581532
N4	-2.5023413438	0.0312249039	2.0944326878
C5	-2.0030462193	0.0987020618	0.8498536982
C6	-4.3144647419	0.3665572626	0.6658722545
H7	-4.8341747845	-0.5750395662	0.4426846826
H8	-4.9419479358	1.1961930881	0.3304436120
C9	-3.9081825755	0.4701284814	2.1316405508
H10	-3.9566950466	1.5020969676	2.5107216131
H11	-4.4987287919	-0.1713359008	2.7925224513
C12	-2.7731659732	0.6226835783	-1.3881186838
C13	-2.1193183458	-0.3539873345	-2.1473599762
C14	-1.7347189220	-0.0800446006	-3.4625136785
H15	-1.2141743730	-0.8412674772	-4.0386789851
C16	-2.0289114364	1.1617113546	-4.0213067194
C17	-2.6983453766	2.1226418869	-3.2602619993
H18	-2.8970748964	3.1038252249	-3.6875164577
C19	-3.0733278416	1.8880478556	-1.9328731370
C20	-3.6799246738	2.9814485782	-1.1100837996
H21	-4.7705548341	2.8886887119	-1.0238170485
H22	-3.4742115301	3.9565746896	-1.5585563746
H23	-3.2512714978	2.9868610859	-0.1009980182
C24	-1.6667870326	0.1087332888	3.2515749109
C25	-1.2587176665	-1.0716060582	3.8955192625
C26	-0.3621936457	-0.9401590217	4.9662532834
H27	-0.0146675185	-1.8419533748	5.4674996441
C28	0.0960444276	0.3090034577	5.3853534410
C29	-0.3400333796	1.4696717373	4.7418244154
H30	0.0257312757	2.4440969998	5.0533060801
C31	-1.2247174006	1.3665481704	3.6691666335
C32	-1.7185462435	-2.4152049419	3.4281682430
H33	-1.4465882847	-3.1944700531	4.1449080883
H34	-1.2709741740	-2.6684149783	2.4575321777
H35	-2.8038113651	-2.4440527632	3.2816142983
C36	1.0349812872	-0.1003721318	1.5196034141
H37	0.8019406919	0.4366499429	2.4487623134
C38	2.2952398956	-0.7878343029	1.4405357346
C39	3.1153758028	-1.0505313144	2.5585411518
H40	2.8258622018	-0.6624586398	3.5336065875
C41	4.2553953414	-1.8321368844	2.4102810967
H42	4.8818862241	-2.0545107906	3.2700719145
C43	4.5911979616	-2.3518653381	1.1514436651
H44	5.4803902097	-2.9687536273	1.0439791404
C45	3.8035020067	-2.0789208101	0.0318533031
H46	4.0814112719	-2.4727857249	-0.9433260106
C47	2.6682319193	-1.2751338258	0.1598873939
C48	1.8084650439	-0.8853290108	-0.9647809691
H49	1.5296164852	-1.6684204985	-1.6693851159
C50	1.5772641983	0.4465968672	-1.3042526974
H51	2.0976722477	1.2646875910	-0.8116081370
H52	1.1230076258	0.6876239855	-2.2637007965
Cl53	-0.5557518049	-2.5552078437	-0.0255432602
H54	0.7986886546	0.3758661314	6.2128305664
H55	-1.7306993930	1.3914666746	-5.0411379491
H56	-1.9219016208	-1.3274244555	-1.7032405116
H57	-1.5254482371	2.2471076525	3.1045075937